NEW ISSUES AND PROBLEMS IN THE DIRAC EQUATION AND THEIR SOLUTIONS

BY

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In the name of Allah, the most gracious, the most merciful

All praise be to Allah for His kindness and guidance, may peace be upon His prophet Mohammed.

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THESIS ABSTRACT

FULL NAME OF STUDENT: AHMAD ABDULWAHAB A. AL-HASAN

TITLE OF STUDY: NEW ISSUES AND PROBLEMS IN THE DIARAC EQUATION AND THEIR SOLUTIONS

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In this thesis, we investigate two issues of current interest in relativistic quantum mechanics. In the first one, we study the Dirac and Klein–Gordon equations with non-central scalar and vector potentials of equal magnitudes. This is done as an attempt to give a proper physical interpretation of this class of problems in which interest has surged recently. The relativistic energy spectra are obtained and shown to differ from those of well-known problems that have the same non-relativistic limit. Consequently, such problems should not be misinterpreted as the relativistic extension of the given potentials. Additionally, we shed new light in some related issues in spin and pseudo-spin symmetry in nuclear physics. In the second topic, we derive a non-relativistic quantum mechanical equation for a system with spatially dependent mass with a unique removal of the ordering ambiguity. This is done by starting from the Dirac equation (with electromagnetic interaction) that does not suffer from this ambiguity and then taking the non-relativistic limit, which is unique. New terms in the Hamiltonian are found, some of which are given physical interpretation.

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في هذه الرسالة سوف ندرس قضيتين لقيتا اهتماما حديثا في ميكانيكا الكم النسبية. في القضية الاولى سوف ندرس معادلتي ديراك وكلاين-جوردن في وجود حقلين غيرمركزيين احدهما قياسي والاخر متجه ولهما نفس المقدار. سنستخدم هذه الدراسة لاعطاء تفسير فيزيائي مقبول لمثل هذه القضايا التي تلقى اهتماما كبيراهذه الايام. سوف نحسب مستويات الطاقة ونبين أنها تختلف عن المستويات المحسوبة لبعض الحقول المعروفة على الرغم أن نهايتهما غير النسبية واحدة. وهكذا فانه لا يمكن تفسير هذه الحلول كتعاميم لهذه الحقول من الحالة غير النسبية إلى الحالة النسبية. بالاضافة الى هذه المسألة فسوف نناقش باختصار مسألة اخرى مرتبطة بها في الفيزياء النووية وهي المسائل التي لها تناظر مغزلي أوشبه مغزلي. في القضية الاخرى من هذه الرسالة سوف نشتق معادلة كمية غير نسبية لجسم له كتلة متغيرة مع المكان مع حل وحيد لمشكلة تعددية الترتيب. سنستخدم لهذا معادلة ديراك (في وجود حقل كهرومغنطيسي) حيث أن هذه المعادلة لا تعاني من مشكلة عدم الوحدانية ومن ثم نحسب النهاية غير النسبية لنحصل على نتيجة وحيدة. سوف نجد بهذه الطريقة حدود جديدة في مؤثر الطاقة وسنعطي لبعضها تفسيرا فيزيائيا.

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CHAPTER 1

INTRODUCTION

The success of quantum mechanics in the description of the atomic and sub-micro world is very impressive and overwhelming. Supplementing that with the theory of Special Relativity created one of the most accurate physical theories in recent history. An example is quantum electrodynamics; the theory that describes the interaction of charged particles with the electromagnetic radiation at high speeds or strong coupling. The Dirac and Klein-Gordon (K-G) equations are the most frequently used wave equations for the description of particle dynamics in relativistic quantum mechanics.

P. A. M. Dirac derived his famous equation in 1928. It describes a relativistic particle of spin one-half at high velocities (below the threshold of pair production). It is a first order matrix linear differential equation whose solution is a 4-component wavefunction (a spinor). Nevertheless, it was hard to find nontrivial exact solutions of this equation. A nontrivial exact solution of the Dirac equation is a solution that, in the non-relativistic limit, reproduces a known solution of the Schrödinger equation with a specific potential. It is customary to refer to such a solution as a "Dirac-Potential" where "potential" is replaced by the name of the corresponding potential in the above-mentioned Schrödinger solution.

Until 1989, there was only one nontrivial exact solution of the Dirac equation concerning the important Coulomb problem. In 1989, Moshinsky and Szczepaniak were able to formulate and solve the oscillator problem (Dirac-Oscillator) [1].

Recently, Alhaidari has introduced an effective approach to the solution of the Dirac equation for spherically symmetric potentials [2-6]. His method was initiated by the observation that different potentials can be grouped into classes; for example, the non-relativistic Coulomb, oscillator and S-wave Morse problems constitute one such class. Therefore, the solution of two problems in one class implies solution for the remaining one. By this method, the S-wave Dirac-Morse problem was formulated and solved [2].

Using the above-mentioned method, other potentials were treated; of these are Dirac-Scarf, Dirac-Rosen-Morse I & II, Dirac-Poschl-Teller, Dirac-Eckart [3], Dirac-Hulthen, and Dirac-Woods-Saxon potentials [7]. Furthermore, quasi-exactly solvable problems at rest mass energies with power-law relativistic potentials were also investigated following the same procedure [4]. Orthogonal polynomials were also used to find L^2 series solutions of Dirac equation for scattering and bound states [8].

On the other hand, relativistic problems with position-dependent mass were rarely investigated. One such example is the Dirac-Coulomb problem with singular mass [9].

In 2005, Alhaidari introduced a systematic method for separating the variables in the Dirac equation [10]. This lead to the solution of the Dirac-Coulomb problem with Aharonov-Bohm and magnetic monopole potentials and to the solution of the Dirac-Oscillator with non-central electromagnetic field [11-12].

In the following chapters, I study four problems related to the developments mentioned above.

In the first problem, I study the three-dimensional Dirac and Klein-Gordon equations with scalar, $S(t,\vec{r})$, and vector, $V(t,\vec{r})$, potentials of equal magnitudes [13]. That is, with $V=\pm S$. This class of problems has recently received an accumulating interest. In my study, I consider a more generalized problem where the potentials are non-central such that the Dirac equation is completely separable in spherical coordinates. The wave functions and their energy spectra will be calculated analytically. To give a clear illustration of my findings in the first study, I will restrict these general cases to the following three well known potentials: Coulomb, Oscillator and Hartmann potentials.

The relativistic energy spectra for these potentials except for the Hartmann potential were previously calculated using other methods from the current equal scalar-vector scenario. By comparing the solutions of both methods, I will show that the energy spectra found by the equal scalar-vector technique disagree with those found by the other well-established methods. However, by taking the non-relativistic limits of the solutions found by both methods, I found that both energy spectra agree with the known non-relativistic results.

These three examples are sufficient to show that even though the method of equal scalar-vector reproduces the correct non-relativistic energy spectra, its relativistic extension should not be misinterpreted as relativistic generalizations for the non-relativistic potentials. As can be seen one non-relativistic potential might result from two

different relativistic formulations, which is compatible with the view that although the non-relativistic limit is well defined and unique; the relativistic extension is not.

In the second problem, I study for the sake of completeness, the S-wave Klein-Gordon-Morse problem with uneven mix of scalar and vector potentials. That is, I take $S(\vec{r}) = \eta V(\vec{r})$ where $\eta \neq \pm 1$. In this case, I will show analytically that, under some physical constraints, the correct relativistic extension of the S-wave Dirac-Morse problem is found [2].

The third problem is related to the problems cited above. These are problems with, what is called, spin and pseudo-spin symmetries and are widely used in nuclear structure studies [14]. As in my first study, I will treat the Dirac equation coupled to a scalar and vector potentials. However, in this case $V(t,r) \pm S(t,r) = \eta$, a real constant. The case with the positive sign is said to have pseudo-spin symmetry while the case with the negative sign is said to have spin symmetry. I will show that the solutions for the case of equal scalar and vector potentials can be easily generalized to the cases with spin and pseudo-spin symmetries. However, it is worth remembering that the problem of the physical interpretation mentioned in the case of equal scalar and vector potentials does not apply for the spin and pseudo-spin symmetric cases. This due to the fact that these last cases are not intended to give relativistic extensions of established problems but are meant to explain the discrepancies in nuclear spectra due to relativistic effects.

In the fourth and last problem of this work, I will study the non-relativistic limit of Dirac equation coupled to a general electromagnetic field. However, the mass of the

particle will be spatially dependent. Position dependent mass (a.k.a. effective mass) is a very useful model in various condensed matter physics problems like hetero-structures, quantum wells, etc [15]. The need for the Dirac equation in such studies stems from the fact that the Schrödinger equation structure contains ambiguity for position dependent mass. This can be seen for example by looking at the Schrödinger equation:

$$\frac{1}{2m}\vec{p}^{\,2}\psi(\vec{r})-\left[E-V(\vec{r})\right]\psi(\vec{r})=0 \tag{1.1}$$

Now it is obvious that when mass is position dependent, the first term (the kinetic operator) in Eq. (1.1) is not uniquely defined. This is because $\vec{p}$ and $m(\vec{r})$ do not commute. It is actually possible to write more than one expression (like $\frac{1}{2}\vec{p}\cdot\frac{1}{m(\vec{r})}\vec{p}$ or $\frac{1}{2\sqrt{m(\vec{r})}}\vec{p}\cdot\frac{1}{\sqrt{m(\vec{r})}}\vec{p}$, or more precisely a Hermitian combination of them) for this term such that they all reproduce the same expression as in Eq. (1.1) for the case of constant mass. A resolution of this difficulty will be sought with the help of the Dirac equation which does not suffer from this problem. I will use the Foldy-Wouthuysen transformation to find the non-relativistic limit to fourth order in the Compton wavelength ($\propto 1/c$, in atomic units). The first result of this reduction will be the derivation of the kinetic energy operator. This method was first used by Cavalcante, et al [16] to find the kinetic energy operator in the case of position-dependent mass. However, I will make a more systematic investigation and re-derive their result. At the same time, I will find a *new term* they missed in their paper. This term can be written in the following form (see Subsection

5.3.2 for an explanation of the symbols):

$$\frac{i}{4m^2}\Sigma\cdot(\vec{p}m)\times\left(\vec{p}-\frac{e}{c}\vec{A}\right)\beta \tag{1.2}$$

The resulting total Hamiltonian will be important when studying small relativistic corrections where the full relativistic equation, with its complexity, is not required.

A final word concerns units that will be used in the following chapters. As in most theoretical studies, natural units will be applied except if otherwise stated. In these units $\hbar = 1$, $e = 1$ and $c = 1$. However, in Chapter 5 where it is essential to keep track of c for taking the non-relativistic limit, we use the atomic units ($\hbar = m = e = 1$) in which c is not constant but goes to infinity.

CHAPTER 2

REVIEW OF NON-RELATIVISTIC QUANTUM MECHANICS AND THE SPECIAL THEORY OF RELATIVITY

2.1. Space Symmetry and Non-Relativistic Physics

Symmetries in physical theories imply conservation of special physical quantities and vice versa [17-19]. They also lead to invariance of the physical system under specific transformations. One such symmetry is that of space and time translation and space rotation. It basically states that if one performs an experiment on a closed physical system then translating the lab in space ($\vec{r} \to \vec{r} + \vec{a}$), in time ($t \to t + \tau$), or rotating it in space ($\vec{r} \to \vec{\theta} \times \vec{r}$) will produce the same results. $\{\tau, \vec{a}, \vec{\theta}\}$ are real transformation parameters. At present, we will ignore the Galilean boosts where the lab moves with constant velocity. It is well-known that these imply the conservation of linear momentum, energy, and angular momentum, respectively. That is, $\Delta\vec{P} = 0$, $\Delta E = 0$, and $\Delta\vec{L} = 0$. To study the properties of the system with these symmetries one defines objects that represent the system and identify the action on the system that correspond to the conserved quantities. For example, one can define local objects such as "scalars", $\phi(t, \vec{r})$ and "vectors" $\vec{A}(t, \vec{r})$

with the properties that under the transformations stated above they change according to the following

$$\phi'(t,\vec{r}') = \phi(t,\vec{r}) \tag{2.1}$$

$$\phi'(t',\vec{r}) = \phi(t,\vec{r}) \tag{2.2}$$

$$A_i'(t,\vec{r}') = R_{ij}A_j(t,\vec{r}) \text{ , such that } \left|\vec{A}'\right| = \left|\vec{A}\right| \tag{2.3}$$

$$\vec{A}'(t',\vec{r}) = \vec{A}(t,\vec{r}) \tag{2.4}$$

where $i = 1,2,3$ and repeated indices are summed over. The invariance of the magnitude of the vector in (2.3) implies that the 3×3 rotation matrix R is orthogonal. That is, $R^T R = 1$. Making infinitesimal transformations (i.e., taking the parameters $\vec{a}$, τ, and $\vec{\theta}$ very small) we obtain from Eqs. (2.1) and (2.2) for the scalar case the following

$$\delta\phi \sim -\mathrm{i}\,\vec{a}\cdot\vec{\nabla}\phi \tag{2.5}$$

$$\delta\phi \sim \mathrm{i}\,\tau\frac{\partial}{\partial t}\phi \tag{2.6}$$

$$\delta\phi \sim -\mathrm{i}\,\vec{\theta}\cdot(\vec{r}\times\vec{\nabla})\phi \tag{2.7}$$

This implies that the operators that correspond to the linear momentum, energy, and angular momentum are, respectively,

$$\hat{P} = -\mathrm{i}\alpha\vec{\nabla} \tag{2.8}$$

$$\hat{H} = \mathrm{i}\alpha\frac{\partial}{\partial t} \tag{2.9}$$

$$\hat{L} = -\mathrm{i}\alpha(\vec{r}\times\vec{\nabla}) \tag{2.10}$$

Where α is a universal constant parameter that has the dimension of the angular momentum. In fact, it is just the Planck constant $\hbar$. Doing the same for the vector field $\vec{A}(t,\vec{r})$ in Eqs. (2.3) and (2.4), leads to the same operator realization for $\hat{P}$ and $\hat{H}$. However, as for the angular momentum the result is

$$\hat{J} = \hat{L} + \hat{S} \tag{2.11}$$

Where $\hat{S}_k = \varepsilon_{kij}\sigma_{ij} = \frac{\mathrm{i}}{4}\varepsilon_{kij}[\sigma_i, \sigma_j]$ and $\{\sigma_i\}_{i=1}^{3}$ are 3×3 Hermitian matrices satisfying the anti-commutation relation $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$. $\hat{L}$ is the orbital part of the total angular momentum $\hat{J}$, and $\hat{S}$ is the spin part. One can show that the algebra obtained by the seven operators $\{\hat{H}, \hat{P}_i, \hat{L}_i\}_{i=1}^{3}$ closes under commutation into the following seven-dimensional Lie algebra:

$$[\hat{P}_i, \hat{P}_j] = 0,\ [\hat{L}_i, \hat{L}_j] = -\mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k,\ [\hat{L}_i, \hat{P}_j] = -\mathrm{i}\hbar\varepsilon_{ijk}\hat{P}_k,$$

$$[\hat{H}, \hat{P}_i] = [\hat{H}, \hat{L}_i] = 0. \tag{2.12}$$

2.1.1. The Free Schrödinger Equation

The first three relations in the set of equations (2.12) constitute the algebra of rotations and translations in 3-dimensional Euclidean space. This algebra has two Casimir operators. That is, there are two invariant operators commuting with all the elements of this algebra corresponding to conserved physical quantities. These two operators are $\hat{P}^2$

and $\hat{L}^2$. Therefore, the whole algebra in Eq. (2.12) has a set of three mutually commuting operators $\left\{\hat{H}, \hat{P}^2, \hat{L}^2\right\}$. Thus, in the scalar case, for example, we can write

$$\hat{H}\phi = \text{const.}\phi \tag{2.13}$$

$$\hat{P}^2\phi = \text{const.}\phi \tag{2.14}$$

$$\hat{L}^2\phi = \text{const.}\phi \tag{2.15}$$

In fact, these are just the well-known results that:

$$\hat{H}\phi = E\phi \tag{2.16}$$

$$\hat{P}^2\phi = 2m\,E\,\phi \tag{2.17}$$

$$\hat{L}^2\phi = \hbar^2\ell(\ell+1)\phi \tag{2.18}$$

Here m is the mass of the particle, E is its energy, and ℓ is the angular momentum quantum number. Eqs. (2.16) and (2.17) give the linear partial differential equation

$$i\hbar\frac{\partial}{\partial t}\phi(t,\vec{r}) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\phi(t,\vec{r}) \tag{2.19}$$

This is nothing but the Schrödinger equation for a free particle. The wave function ϕ, which is generally a complex quantity, contains all the physics of the system like the probability distribution (square of the absolute value of the wave function) and the energy spectrum. In the following subsection, interaction in the Schrödinger equation will be introduced via two alternative approaches. It should be noted that a momentum-linearized version of the time independent Schrödinger equation (2.17) can be obtained by "taking its square root". That is, one could obtain an equation that is linear in the momentum by

writing

$$\gamma_i \hat{P}_i \phi = \pm\sqrt{2mE}\,\phi \tag{2.20}$$

This is possible only if $\{\gamma_i\}_{i=1}^{3}$ are matrices satisfying the anti-commutation relations $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$. The minimum dimension for these matrices is 2×2. In that case, they become the three Pauli spin matrices and Eq. (2.20) could be used as a non-relativistic model for describing spinors.

2.1.2. The Schrödinger Equation with Interaction

The interaction can be introduced in the free Schrödinger equation using either one of two approaches. In the first approach, called the "potential approach", we use the operator representations obtained in Eqs. (2.8-10) to postulate the quantum analog of the classical energy conservation equation $H = \frac{1}{2m}\vec{P}^2 + V$. That is,

$$i\hbar\frac{\partial}{\partial t}\psi(t,\vec{r}) = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(t,\vec{r})\right]\psi(t,\vec{r}) \tag{2.21}$$

Where $V(t,\vec{r})$ is a real potential function. This is the celebrated time-dependent Schrödinger equation. In many cases, the Hamiltonian is time-independent which makes it possible to separate time from Eq. (2.21) by the substitution:

$$\psi(t,\vec{r}) = e^{-iEt}\psi(\vec{r}) \tag{2.22}$$

Putting this back into Eq. (2.21) leads to the time-independent Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(r)\right]\psi(\vec{r}) = E\psi(\vec{r}) \tag{2.23}$$

Solving this equation is enough to calculate the physical properties of the system like its energy, probability distribution, currents, etc. These considerations can be found in any standard quantum mechanics book [20-23].

In the second approach, called the "*gauge invariance*" approach, we introduce another type of symmetry for the system. It is different from the space symmetry given by Eqs. (2.1-2). It is a local symmetry and could be thought of as an internal symmetry for the particle that carries a "charge" associated with this symmetry (e.g., electric charge, weak-interaction charge, strong-color charge, etc.). A "gauge" vector field $\vec{A}(\vec{r})$ that couples to the particle and interacts with it, is introduced such that the interaction is invariant under the following "gauge transformation":

$$\phi'(\vec{r}) = e^{\mathrm{i}q\lambda(\vec{r})}\phi(\vec{r}),\ \vec{A}'(\vec{r}) = \vec{A}(\vec{r}) + \vec{\nabla}\lambda(\vec{r}) \tag{2.24}$$

Where $\lambda(\vec{r})$ is a real function and q is the real charge parameter (the coupling constant). Therefore, replacing the gradient operator $\vec{\nabla}$ in the free Schrödinger equation (2.19) by $\vec{\nabla} - \mathrm{i}\,q\,\vec{A}(\vec{r})$ (i.e. $\hat{P} \to \hat{P} - \hbar\,q\,\vec{A}$) gives the following gauge invariant equation

$$i\hbar\frac{\partial}{\partial t}\phi(t,\vec{r}) = -\frac{\hbar^2}{2m}\left[\vec{\nabla} - \mathrm{i}\,q\,\vec{A}(\vec{r})\right]^2\phi(t,\vec{r}) \tag{2.25}$$

This equation describes the interaction of the particle with the gauge field $\vec{A}(\vec{r})$. Under space transformation, this gauge field transforms according to Eqs. (2.3-4).

2.1.3. Exact Solution of the Schrödinger Equation for Practical Potentials

Given the Hamiltonian (or equivalently the potential), Eq. (2.23) can in principle be solved. In general, this equation is a second order partial differential equation. Its complete solution requires boundary conditions. The wavefunction for bound states, for example, is finite at the origin and vanishing at infinity. These boundary conditions lead to quantization rules that dictate the form of the energy spectrum. The Schrödinger equation was solved exactly for many practical potentials. These include the Coulomb potential (the hydrogen-like atom), the 3D anisotropic harmonic oscillator and others [20-23]. A list of some of the potentials that have been exactly solved can be found in [24].

2.1.4. Limitations of the Schrödinger Equation

Firstly, the Schrödinger equation is non-relativistic. It is actually invariant under a larger transformation group (the Galilean group), which is larger than that described in Section 2.1. This means that for relativistic particles, the Schrödinger equation is not applicable and therefore a different equation is required. A guide for resolving this difficulty is to use a symmetry group for space-time rather than that of space and time separately (or the larger Galilean group). A second limitation of the Schrödinger equation is the absence of spin (other than spin 1 described in Section 2.1 by Eqs. (2.3-4) which is essential to understand physical phenomena like splitting of spectral lines. A last

important observation relating to the Schrödinger equation is in the kinetic part of Eq. (2.21). When mass is position dependent, then it is not obvious what will be the form of the kinetic part due to the fact that position and linear momentum do not commute. Notice that replacing the mass m in Eq. (2.21) by $m(\vec{r})$ is not enough because the resulting operator is not Hermitian. In the following sections, space-time symmetry will be applied to derive relativistic equations that can handle the problems cited above.

2.2. Space-Time Symmetry: The Relativistic Equation

In relativistic physics, space and time are combined in one non-Euclidean continuum called space-time. The physical symmetry group of this space-time is the Poincare group (again excluding inversion and time reversal) that is equivalent to Lorentz group plus space-time translation. The coordinates are given by the four-vector $(ct, x, y, z) = (x^0, x^1, x^2, x^3)$, where c is the speed of light. In compact form these coordinates are abbreviated as x^μ for $\mu = 0,1,2,3$. The metric of space-time is $g_{\mu\nu} = (1,-1,-1,-1)$ or $g^{\mu\nu} = (1,-1,-1,-1)$. Raising or lowering indices is given for a four-vector by $V_\mu = g_{\mu\nu}V^\nu$ and $V^\mu = g^{\mu\nu}V_\nu$. Obvious relations hold for other types of fields [25].

2.2.1. Poincaré Group

In Section 2.1, we found the algebra of space translations and rotations, in three-dimensional Euclidean space, in addition to the translation in time. The operator elements of this 7-dimenional algebra are given by Eqs. (2.8-10) and their algebra by Eq. (2.12). The Poincaré algebra, on the other hand, has ten generators given by the momentum four-vector p_μ, the angular momentum three-vector J_i and the three generators of Lorentz boost N_i. It is the algebra of translation and rotation in the four-dimensional Minkowski space whose coordinates are x^μ and whose metric is $g_{\mu\nu}$. The associated group (the Poincaré group) is the proper symmetry group for the description of particles with high speeds comparable to that of light. The last two types of generators can be combined into one anti-symmetric tensor $J_{\mu\nu}$ that has six elements such that $J_{ij} = \varepsilon_{ijk} J_k$ and $J_{i0} = N_i$. Together, the momentum and the anti-symmetric tensor obey the following algebra:

$$[p_\mu, p_\nu] = 0\,,\ [J_{\mu\nu}, J_{\rho\sigma}] = i\hbar\left(g_{\nu\rho}J_{\mu\sigma} - g_{\mu\rho}J_{\nu\sigma} + g_{\mu\sigma}J_{\nu\rho} - g_{\nu\sigma}J_{\mu\rho}\right),$$

$$[J_{\mu\nu}, p_\alpha] = i\hbar\left(g_{\alpha\nu}p_\mu - g_{\alpha\mu}p_\nu\right) \qquad (2.26)$$

Irreducible representations of this group are classified according to their mass and spin. This follows from the fact that Poincare group has two Casimir operators (operators commuting with all generators of the group): p^2 and W^2, where $W^\mu = \frac{1}{4!}\varepsilon^{\mu\nu\alpha\beta}P_\nu J_{\alpha\beta}$. This means that in one irreducible representation of the group, both of these quantities are

fixed. It can be shown that $p^2 = m^2c^2$ (continuous) and $W^2 = \hbar^2 m^2 c^2 s(s+1)$ where $s \in \{0, 1/2, 1, 3/2, ...\}$ and m is the rest mass of the particle. Examples of these representations are a scalar particle with zero spin, and a spinor with one-half spin. Manipulation of the algebra in Eq. (2.26), leads to invariant equation of motion depending on the invariant properties of the irreducible representation [26-27].

2.2.2. The Free Klein-Gordon Equation

As mentioned above, a scalar function represents a spin zero particle. It is governed by the following invariant Klein-Gordon equation:

$$p^\mu p_\mu \phi(x^\nu) - m^2 \phi(x^\nu) = 0 \;\rightarrow\; \partial^\mu \partial_\mu \phi(x^\nu) + m^2 \phi(x^\nu) = 0 \tag{2.27}$$

where we have adopted the conventional relativistic units $\hbar = c = 1$. It is invariant under the Poincare group. This equation can be seen to result from the fact that p^2 is a Casimir operator equal to a constant, m^2. As for the Schrödinger equation, p_μ in configuration space is represented by $-i\dfrac{\partial}{\partial x^\mu}$.

2.2.3. The Free Dirac Equation

It is possible to apply to Eq. (2.27) a momentum-linearization procedure similar to that

which was introduced at the end of Subsection 2.1.1 in the non-relativistic theory. That is, we can write the following relativistically invariant equation for the spinor wave function:

$$\left(\gamma^{\mu} p_{\mu} + m\right)\psi(x^{\nu}) = 0 \;\rightarrow\; \left(-i\gamma^{\mu}\partial_{\mu} + m\right)\psi(x^{\nu}) = 0 \tag{2.28}$$

Consequently, γ^{μ} are four matrices that should satisfy the anti-commutation relations $\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu}$. Equation (2.28) is the Dirac equation for a free spinor particle.

2.2.4. Gauge Invariant Coupling

Eqs. (2.27) and Eq. (2.28) are written for free particles. Introducing an interaction must not destroy the relativistic invariance of the equations. One way to introduce the interaction is through another type of invariance, the gauge invariance. Gauge invariance, which was introduced in Subsection 2.1.2, means that the equation is invariant under a local phase transformation. This requires the introduction of a four-vector that has a special transformation property. As an example, take the scalar field $\phi(x)$. The local phase transformation has the form:

$$\phi'(x) = e^{-i\alpha(x)}\phi(x) \tag{2.29}$$

Notice that this gauge transformation does not affect the coordinates. Now introduce the four-vector $A_{\mu}(x)$ that transforms under gauge transformation as:

$$A'_\mu(x) = A_\mu(x) + \frac{\partial}{\partial x^\mu}\alpha(x) \tag{2.30}$$

To introduce the interaction, make the substitution (minimal substitution) $p_\mu \rightarrow p_\mu + A_\mu$.

Eqs. (2.15-16) become:

$$(\partial^\mu + iA^\mu)(\partial_\mu + iA_\mu)\phi(x^\nu) - m^2\phi(x^\nu) = 0 \tag{2.31}$$

$$\left[-i\hbar\gamma^\mu(\partial_\mu + iA_\mu) + m\right]\psi(x^\nu) = 0 \tag{2.32}$$

These are Klein-Gordon and Dirac equations for particles interacting with a gauge field (such as an electromagnetic field).

CHAPTER 3

THE DIRAC EQUATION

3.1. The Free Dirac Equation

The Dirac equation was formulated by P. A. M. Dirac in 1928 to generalize the Schrödinger equation and to overcome the shortcomings of the Klein-Gordon equation (as they were understood at the time) [28]. It describes a relativistic particle with spin one-half whose wave function is a four-component spinor. It can be written in the following covariant form:

$$\left(i\gamma^{\mu} \frac{\partial}{\partial x^{\mu}} - m \right) \psi(x) = 0 \tag{3.1}$$

Where the spinor is $\psi(x) = \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \\ \psi_4(x) \end{bmatrix}$. The matrices γ^{μ} are constant matrices satisfying the relation:

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu} \tag{3.2}$$

They can be represented in more than one equivalent representation. A familiar representation is given by the Pauli representation:

$$\gamma^0 = \beta, \ \gamma^i = \beta\alpha_i \tag{3.3}$$

Where $i = 1,2,3$ while β and α_i are given by:

$$\beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \ \alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} \tag{3.4}$$

Here the non-vanishing entries are 2×2 matrices and σ_i are the more familiar Pauli matrices given by:

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{3.5}$$

Eq. (3.1) is the free Dirac equation. It can be written in terms of the Dirac Hamiltonian:

$$i\frac{\partial}{\partial t}\psi(\vec{r},t) = \left(\vec{\alpha}\cdot\vec{p} + m\beta\right)\psi(\vec{r},t) \equiv H_0\psi(\vec{r},t) \tag{3.6}$$

The free Hamiltonian H_0 is given in detail by the following 4×4 matrix:

$$H_0 = \begin{bmatrix} m & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -m \end{bmatrix} \tag{3.7}$$

Where all entries are 2×2 matrices. There is more than one way to introduce an interaction into this free Hamiltonian. This is reviewed in the following section.

3.2. Potential Coupling in the Dirac Equation

The fact that the Dirac equation (similarly the Klein-Gordon equation) for free particles is constructed using two objects: the four-vector linear momentum operator $p_\mu = i\frac{\partial}{\partial x^\mu}$ and the scalar rest mass m, allows one to introduce naturally two types of

potential coupling. In fact, by introducing fields with different properties makes it possible to classify at least six kinds of coupling. These will be treated in this section restricting them to be static.

3.2.1. Minimal Substitution: Vector Coupling

This is a gauge invariant coupling to a four-vector using the minimal substitution:

$$p_\mu \rightarrow p_\mu + A_\mu \ , \ A_\mu = (\phi, -\vec{A}) \tag{3.8}$$

The new Dirac Hamiltonian becomes:

$$H = \begin{bmatrix} m + A_0 & -i\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{A} \\ -i\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{A} & -m + A_0 \end{bmatrix} \tag{3.9}$$

This four-vector can represent an electromagnetic field if the electric and magnetic fields are given by:

$$\vec{E} = -\frac{\partial}{\partial t}\vec{A} - \vec{\nabla}\phi \ , \quad \vec{B} = \vec{\nabla}\times\vec{A} \tag{3.10}$$

3.2.2. Pseudo-Four-Vector Coupling

Similar to the vector coupling, this coupling is introduced via the substitution $p_\mu \rightarrow p_\mu + \gamma_5 B_\mu$ where $(B_0, \vec{B})$ is a four-vector potential and $\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

(the 1 is a 2×2 matrix). This coupling gives the following Hamiltonian (including the previous one):

$$H=\begin{bmatrix} m+A_0+\vec{\sigma}\cdot\vec{B} & -i\vec{\sigma}\cdot\vec{\nabla}+\vec{\sigma}\cdot\vec{A}+B_0 \\ -i\vec{\sigma}\cdot\vec{\nabla}+\vec{\sigma}\cdot\vec{A}+B_0 & -m+A_0+\vec{\sigma}\cdot\vec{B} \end{bmatrix} \tag{3.11}$$

3.2.3. Three-Vector Coupling

This is introduced through the substitution $\vec{p}\rightarrow\vec{p}-i\vec{W}\gamma_0$, where $\vec{p}$ is the linear momentum three-vector operator and $\vec{W}(\vec{r})$ is a three-vector. This leads to:

$$H=\begin{bmatrix} m+A_0+\vec{\sigma}\cdot\vec{B} & -i\vec{\sigma}\cdot\vec{\nabla}+\vec{\sigma}\cdot\vec{A}+B_0+i\vec{\sigma}\cdot\vec{W} \\ -i\vec{\sigma}\cdot\vec{\nabla}+\vec{\sigma}\cdot\vec{A}+B_0-i\vec{\sigma}\cdot\vec{W} & -m+A_0+\vec{\sigma}\cdot\vec{B} \end{bmatrix} \tag{3.12}$$

3.2.4. Pseudo-Three-Vector Coupling

Similar to the three-vector coupling, the pseudo-three-vector coupling is produced via the substitution $\vec{p}\rightarrow\vec{p}+\vec{U}\gamma_5\gamma_0$, where $\vec{U}$ is a static potential. The new Hamiltonian reads:

$$H=\begin{bmatrix} m+A_0+\vec{\sigma}\cdot\vec{B}+\vec{\sigma}\cdot\vec{U} & -i\vec{\sigma}\cdot\vec{\nabla}+\vec{\sigma}\cdot\vec{A}+B_0+i\vec{\sigma}\cdot\vec{W} \\ -i\vec{\sigma}\cdot\vec{\nabla}+\vec{\sigma}\cdot\vec{A}+B_0-i\vec{\sigma}\cdot\vec{W} & -m+A_0+\vec{\sigma}\cdot\vec{B}-\vec{\sigma}\cdot\vec{U} \end{bmatrix} \tag{3.13}$$

3.2.5. Scalar Coupling

This simple coupling is done by introducing a scalar $S(\vec{r})$ through the replacement $m \to m + S(\vec{r})$ leading to:

$$H = \begin{bmatrix} m + A_0 + \vec{\sigma}\cdot\vec{B} + \vec{\sigma}\cdot\vec{U} + S & -i\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{A} + B_0 + i\vec{\sigma}\cdot\vec{W} \\ -i\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{A} + B_0 - i\vec{\sigma}\cdot\vec{W} & -m + A_0 + \vec{\sigma}\cdot\vec{B} - \vec{\sigma}\cdot\vec{U} - S \end{bmatrix} \tag{3.14}$$

3.2.6. Pseudo-Scalar Coupling

Replacing the mass m by $m + i\gamma_5 T(\vec{r})$ (pseudo-scalar coupling) leads to:

$$H = \begin{bmatrix} m + A_0 + \vec{\sigma}\cdot\vec{B} + \vec{\sigma}\cdot\vec{U} + S & -i\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{A} + B_0 + i\vec{\sigma}\cdot\vec{W} + iT \\ -i\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{A} + B_0 - i\vec{\sigma}\cdot\vec{W} - \mathrm{i}T & -m + A_0 + \vec{\sigma}\cdot\vec{B} - \vec{\sigma}\cdot\vec{U} - S \end{bmatrix} \tag{3.15}$$

In the following chapters, use will be made of some of these couplings.

3.3. Exact Solution of the Dirac Equation

In this section, some exact solutions of the Dirac equation will be reviewed. This includes non-central potentials in addition to the spherically symmetric cases. These will

be needed in Chapter 6, where I will compare them with our new findings.

3.3.1. Solution for Central Potential

For problems with central potentials, both the square of the total angular momentum J^2 and its z-component J_z commute with the Hamiltonian and with themselves. This means that it is possible to find a common eigen-function of the three operators [21-23, 29-31]. For a Hamiltonian H and wave function $\psi(\vec{r},t)$, the solution will satisfy the following equations:

$$H\psi(\vec{r},t) = E\psi(\vec{r},t) \tag{3.16}$$

$$J^2\psi(\vec{r},t) = j(j+1)\psi(\vec{r},t) \tag{3.17}$$

$$J_z\psi(\vec{r},t) = M\psi(\vec{r},t) \tag{3.18}$$

For time independent Hamiltonian, time can be separated by defining

$$\psi(\vec{r},t) = e^{-iEt}\psi(\vec{r}) \tag{3.19}$$

The two angular equations (3.17) and (3.18) are satisfied by the following two solutions depending on the value of the orbital angular momentum l:

$$\psi(\vec{r}) = \frac{1}{r}\begin{bmatrix} \left(\frac{l+M+1/2}{2l+1}\right)^{1/2} Y_l^{M-1/2}(\theta,\varphi) f(r) \\ \left(\frac{l-M+1/2}{2l+1}\right)^{1/2} Y_l^{M+1/2}(\theta,\varphi) f(r) \\ \left(\frac{l-M+3/2}{2l+3}\right)^{1/2} Y_{l+1}^{M-1/2}(\theta,\varphi) g(r) \\ -\left(\frac{l+M+3/2}{2l+3}\right)^{1/2} Y_{l+1}^{M+1/2}(\theta,\varphi) g(r) \end{bmatrix}, \; l = j - 1/2 \tag{3.20}$$

$$\psi(\vec{r}) = \frac{1}{r}\begin{bmatrix} \left(\frac{l-M+1/2}{2l+1}\right)^{1/2} Y_l^{M-1/2}(\theta,\varphi) f(r) \\ -\left(\frac{l+M+1/2}{2l+1}\right)^{1/2} Y_l^{M+1/2}(\theta,\varphi) f(r) \\ \left(\frac{l+M-1/2}{2l-1}\right)^{1/2} Y_{l+1}^{M-1/2}(\theta,\varphi) g(r) \\ -\left(\frac{l-M-1/2}{2l-1}\right)^{1/2} Y_{l+1}^{M+1/2}(\theta,\varphi) g(r) \end{bmatrix}, \; l = j + 1/2 \tag{3.21}$$

Where Y_l^m are the spherical harmonics. Substituting Eq. (3.20) or Eq. (3.21) back into Eq. (3.16) leads to a radial equation. The form of this equation depends on the form of the potential. For example if the Dirac equation is coupled to a four-vector (see Eq. 3.9) with vanishing space-like component $(\vec{A} = 0)$ and $(A_0 = A_0(r))$ then Eq. (3.16) becomes:

$$(E + A_0 - m) f = -i\left(\frac{d}{dr} + \frac{k}{r}\right) g \tag{3.22}$$

$$(E + A_0 + m) g = -i\left(\frac{d}{dr} - \frac{k}{r}\right) f \tag{3.23}$$

These are two coupled first order differential equations. Solving one equation for one function (f or g) and substituting into the other equation gives a second order

differential equation that can be solved by the usual methods [32]. Applying boundary conditions will dictate the form of the energy spectrum.

Therefore, the main requirement in central potential problems is to solve the radial Dirac equation. Of course, not all types of potentials or couplings are exactly solvable. Thus, a new technique was introduced [2-6].

The central idea in the approach is to transform the two coupled first order differential equations resulting from the radial Dirac equation to Schrödinger-like equations. This makes the two solutions of the relativistic problem easily attainable by simple and direct correspondence with well-known exactly solvable non-relativistic problems. This transformation consists of two processes. The first is a unitary transformation of the Dirac equation that, of course, reduces to the identity in the non-relativistic limit. The second is the introduction, in a natural way, of an extra potential component that is constrained to depend, in a particular way, on the independent potential function of the problem. An important aspect of this approach is the introduction of potential in a non-minimal coupling through the replacement $\vec{A} \to \pm i\vec{A}$ in the lower off diagonal element of the Hamiltonian of Eq. (3.9), giving the Hamiltonian:

$$H = \begin{bmatrix} m + A_0 & -i\vec{\sigma}\cdot\vec{\nabla} + i\vec{\sigma}\cdot\vec{A} \\ -i\vec{\sigma}\cdot\vec{\nabla} - i\vec{\sigma}\cdot\vec{A} & -m + A_0 \end{bmatrix} \tag{3.24}$$

This is acceptable even though in this case the field cannot be interpreted as an electromagnetic field. By this method, the Dirac equation was solved exactly for many practical potentials as can be seen in the list cited at the end of this chapter.

3.3.2. Solution for Non-Central Potential

Recently Alhaidari introduced a systematic and intuitive approach to separate the three dimensional Dirac equation in spherical coordinates [33]. In this approach, the Dirac equation is coupled to a static non-central electromagnetic field (see Section 3.2.1) of the form (in spherical coordinates):

$$A_0(\vec{r}) = V(r),\ A_r(\vec{r}) = W_r(r),\ A_\theta(\vec{r}) = 0,\ A_\phi(\vec{r}) = \frac{W_\theta(\theta)}{r} \tag{3.25}$$

After a lengthy calculation, the complete Dirac equation was then written in the form:

$$\begin{pmatrix} m+V-\varepsilon & -\sigma_3(\partial_r + iW_r) \\ \sigma_3(\partial_r + iW_r) & -m+V-\varepsilon \end{pmatrix} + \frac{1}{r}\begin{pmatrix} 0 & -\sigma_1\partial_\theta - i\sigma_2 W_\theta \\ \sigma_1\partial_\theta + i\sigma_2 W_\theta & 0 \end{pmatrix} + \frac{1}{r\sin\theta}\begin{pmatrix} 0 & -\sigma_2\partial_\phi - i\sigma_1 W_\phi \\ \sigma_2\partial_\phi + i\sigma_1 W_\theta & 0 \end{pmatrix}\Bigg]\begin{pmatrix} g_+ \\ g_- \end{pmatrix} = 0 \tag{3.26}$$

Where $g_\pm = \begin{pmatrix} g_\pm^+ \\ g_\pm^- \end{pmatrix}$. Separating variables as $g_s^\pm(\vec{r}) = R_s^\pm(r)\Theta_s^\pm(\theta)\Phi_s^\pm(\phi)$, where $s = \pm$,

Eq. (3.26) transforms to three decoupled equations as follows:

$$\left(\pm\sigma_2\frac{d}{d\phi} \pm i\sigma_1 W_\phi\right)\Phi_\pm = \pm i\sigma_2\varepsilon_\phi\Phi_\pm \tag{3.27}$$

$$\left(\pm\sigma_1\frac{d}{d\theta} \pm i\sigma_2 W_\theta \pm i\sigma_2\frac{\varepsilon_\phi}{\sin\theta}\right)\Theta_\pm = \sigma_3\varepsilon_\theta\Theta_\pm \tag{3.28}$$

$$\begin{pmatrix} m+V-\varepsilon & \sigma_3\left(-\frac{d}{dr}+\frac{\varepsilon_\theta}{r}-iW_r\right) \\ \sigma_3\left(\frac{d}{dr}+\frac{\varepsilon_\theta}{r}-iW_r\right) & -m+V-\varepsilon \end{pmatrix}\begin{pmatrix} R_+ \\ R_- \end{pmatrix}=0 \tag{3.29}$$

Where ε_θ and ε_ϕ are real separation constants. These were then shown to be exactly solvable for potentials of the form:

$$V(r)=\frac{C}{r},\ W_r=0,\ W_\theta(\theta)=\frac{a-b\cos\theta}{\sin\theta} \tag{3.30}$$

Where a, b and C are constants. These potentials include cases like the Coulomb, Ahranov-Bohm and magnetic monopole potentials.

3.3.3. The Two-Point Green's Function

The Green' function is of prime importance for the calculation of different physical quantities. For example, it can be used to find the wave function at t_2 if it is known at an initial moment t_1. Another use of Green's functions is the calculation of bound energy spectrum. These are found by locating the poles of the Green's function [34-35]. In parallel with the above developments to find exact solution of Dirac equation, the same techniques were used to calculate relativistic Green's functions for some practical potentials [36-38].

This ends a survey of the different methods introduced to exactly solve the Dirac equation. In the following three sections, a review of the solution of the Dirac equation

for three potentials will be discussed. These problems will be needed in Chapter 6 where an attempt will be made to give a proper interpretation of one of the most widely used methods to find exact solution of Dirac equation.

3.3.4. Dirac-Coulomb Problem

This problem was the first non-trivial one to be solved. It was solved by Gordon in 1928 [39]. It is a free Dirac equation coupled to a four-vector (see Section 3.2.1) with the $\vec{A} = 0$ and $\phi = -\frac{Ze^2}{r}$ where e is the proton charge and Z is the atomic number. This is the relativistic generalization of the hydrogen-like atoms. For bound states, the energy spectrum was found to be:

$$E_{nj} = mc^2 \left[1 + \left(\frac{\alpha_0}{n + \sqrt{(j+1/2)^2 - \alpha_0^2}} \right)^2 \right]^{-1/2}, \; n = 0,1,2,.., \; j = 0, 1/2, 1, 3/2, ... \qquad (3.31)$$

$\alpha_0 = Z\alpha = Z\frac{e^2}{c\hbar}$, n is the principle quantum number and j is the total angular momentum. The wave function and its properties can be found in any standard relativistic quantum mechanics book [21-23, 29, 30-31, 39].

3.3.5. Dirac-Oscillator Problem

This was the second Dirac problem that was exactly solved [1, 40]. It took about sixty-one years to find this solution after the celebrated Coulomb case. This is the free Dirac problem coupled to a three-vector $\vec{W} = m\omega\vec{r}$ (see Section 3.2.2). The energy spectrum has the form:

$$E = \left\{mc^2\omega\hbar\left[2(N+1)+\varepsilon(2j+1)\right]+m^2c^4\right\}^{1/2} \text{ (for positive energy)} \tag{3.32}$$

$$E = -\left\{mc^2\omega\hbar\left[2(N+2)+\varepsilon(2j+1)\right]+m^2c^4\right\}^{1/2} \text{ (for negative energy)} \tag{3.33}$$

$N = 0, 1, 2,..$ is the principle quantum number, $j = 0, 1/2, 1,...$ is the total angular momentum, $\varepsilon = \pm 1$ depending on the value of the orbital momentum $l = j \pm 1/2$ and ω is the non-relativistic frequency of the oscillator. Notice the difference between the coupling in this case ($\vec{W} \propto \vec{r}$) and the usual harmonic potential ($V \propto r^2$).

3.3.6. Dirac-Hartmann Problem

The Hartmann potential was introduced in Chemistry to study ring-like molecules [41]. It is non-central and has the general form:

$$V(\vec{r}) = \frac{Z}{r} - \frac{a}{r^2 \sin^2\theta} \tag{3.34}$$

Where Z and a are arbitrary real numbers. There is no conclusive relativistic solution of this problem except the recent one using equal scalar-vectors method [42]. However, it will be shown in chapter four that the method of equal scalar-vector should not be misinterpreted. Thus, this solution is not necessarily the correct relativistic solution. Notice that the Hartman potential reduces to the Coulomb potential if a was taken to be zero.

3.3.7. Other Exact Solutions of the Dirac Equation

As stated above, many other exact solutions of Dirac equation were found using the different methods discussed previously. These problems include the following potentials: S-wave Morse [2], Dirac-Scarf, Dirac-Rosen-Morse I & II, Dirac-Poschl-Teller, Dirac-Eckart [3], Dirac-Hulthen, Dirac-Woods-Saxon [7], Dirac-Coulomb with Aharonov-Bohm and magnetic monopole potential [11] and Dirac-Oscillator with non-central electromagnetic field [12].

CHAPTER 4

THE DIRAC AND KLEIN-GORDON EQUATIONS WITH SCALAR AND VECTOR POTENTIALS

4.1. The Dirac and Klein-Gordon Equations with Equal Scalar and Vector potentials

The fact that the Dirac and Klein-Gordon (K-G) equations, for free particles (see Subsections 2.3.2-3), are constructed using two objects: the four-vector linear momentum operator $p_\mu = i\partial_\mu$ and the scalar rest mass m, allows one to naturally introduce two types of potential coupling. One is the gauge invariant coupling to the four-vector potential $\{A_\mu(t,\vec{r})\}_{\mu=0}^{3}$ which is introduced via the minimal substitution $p_\mu \to p_\mu - gA_\mu$, where g is a real coupling parameter (see Subsection 3.2.1). The other, is an additional coupling to the space-time scalar potential $S(t,\vec{r})$ that is introduced by the substitution $m \to m+S$ (see Subsection 3.2.5). The term "four-vector" and "scalar" refers to the corresponding unitary irreducible representation of the Poincaré space-time symmetry group discussed in Section 2.3. Gauge invariance of the vector coupling allows for the freedom to fix the gauge (eliminate the nonphysical gauge modes) without altering the physical content of the problem. There are many choices of gauge fixing that one could

impose. The Lorentz gauge, $\partial_\mu A^\mu = 0$, and the Coulomb gauge, $\vec{\nabla}\cdot\vec{A} = 0$, are two of the most commonly used conditions. However, many choose to simplify the solution of the problem by taking the space component of the vector potential to vanish (i.e., $\vec{A} = 0$). If we adapt this latter choice and write the time component of the four-vector potential as $gA_0(t,\vec{r}) = V(t,\vec{r})$, then we end up with two independent potential functions in the Dirac and K-G equations. These are the "vector" potential *V* and the scalar potential *S*.

As discussed in Chapters 2 and 3, the free Dirac and K-G equations are written as $\left(i\gamma^\mu\partial_\mu - m\right)\psi_D(t,\vec{r}) = 0$ and $\left(\partial^\mu\partial_\mu + m^2\right)\psi_{KG}(t,\vec{r}) = 0$, respectively. The convention of summing over repeated indices is used. The vector and scalar couplings mentioned above introduce potential interactions by mapping the free Dirac and K-G equations above into the following

$$\left\{\gamma^0\left[i\frac{\partial}{\partial t} - V(t,\vec{r})\right] + i\vec{\gamma}\cdot\vec{\nabla} - m - S(t,\vec{r})\right\}\psi_D(t,\vec{r}) = 0 \tag{4.1}$$

$$\left\{-\left[i\frac{\partial}{\partial t} - V(t,\vec{r})\right]^2 - \vec{\nabla}^2 + [S(t,r)+m]^2\right\}\psi_{KG}(t,\vec{r}) = 0 \tag{4.2}$$

respectively. Recently, interest in the solutions of these two equations for the case where $S(\vec{r}) = \pm V(\vec{r})$ has surged. For the most recent contributions, with citations to earlier work, one may refer to [43] and references therein.

The following sections present a critical investigation of this case, $S = \pm V$, considering the more general situation where the potentials are angular-dependent (non-

central) such that the Dirac and K-G equations are completely separable in spherical coordinates. The target is those studies that present an improper physical interpretation of the solutions of such problems. However, studies that are aimed at the investigation of issues that are relevant to those problems such as the pseudo-spin symmetry in nuclear physics and the effect of the breaking of this symmetry will be mentioned at the end of this chapter. It will be shown (by example) that the solutions of such problems do not coincide with those of well-established problems that have the same non-relativistic limit. The Coulomb, oscillator and Hartmann potentials will be studied. This constitutes a (sufficient) proof that although the non-relativistic limit is well defined and unique; the relativistic extension is not. Thus, the physical interpretation of the relativistic problem should not be confused with those that may have the same non-relativistic spectrum or similar structure of the potential functions. The formulation of the problem will be carried out in the following section whereas illuminating solutions for several examples will be obtained in the section that follows.

4.1.1. Formulation of the Problem and Solution of the Angular Equations

For time-independent potentials we can write the total wave function as $\psi(t,\vec{r}) = e^{-i\varepsilon t}\psi(\vec{r})$, where ε is the relativistic energy. Consequently, the Dirac and K-G equations (4.1) and (4.2) become, respectively

$$\begin{pmatrix} m+S(\vec{r})+V(\vec{r}) & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -m-S(\vec{r})+V(\vec{r}) \end{pmatrix}\begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} = \varepsilon\begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}, \tag{4.3}$$

$$\left\{\vec{\nabla}^2 + [V(\vec{r})-\varepsilon]^2 - [S(\vec{r})+m]^2\right\}\psi_{KG}(\vec{r}) = 0 \tag{4.4}$$

Where ψ_+ (ψ_-) is the top (bottom) two-component spinor of ψ_D. Now, if we take $S = \pm V$, then the potential contribution in the Dirac Hamiltonian will be either $\begin{pmatrix} 2V & 0 \\ 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 \\ 0 & 2V \end{pmatrix}$. It is expected that such a singular potential structure might result in irregular behavior of the solution. Nevertheless, with $S = \pm V$, equation (4.3) gives one spinor component in terms of the other as

$$\psi_{\mp}(\vec{r}) = \frac{1}{\varepsilon \pm m}\left(-i\vec{\sigma}\cdot\vec{\nabla}\right)\psi_{\pm}(\vec{r}) \tag{4.5}$$

where $\varepsilon \neq \mp m$. This equation is referred to as the "kinetic balance" relation. Since $\varepsilon = +m$ ($\varepsilon = -m$) is an element of the positive (negative) energy spectrum of the Dirac Hamiltonian, then this relation with the top (bottom) sign is *not* valid for the negative (positive) energy solutions. Substituting from Eq. (4.5) into the Dirac equation (4.3), with $S = \pm V$, results in the following second order differential equation

$$\left\{\vec{\nabla}^2 - 2(\varepsilon \pm m)V(\vec{r}) + \varepsilon^2 - m^2\right\}\psi_{\pm}(\vec{r}) = 0 \tag{4.6}$$

giving ψ_+ (ψ_-) as an element of the positive (negative) energy solutions. To obtain the other spinor component, we use the kinetic balance relation (4.5) with the top (bottom) sign. Therefore, the choice $S = +V$ ($S = -V$) dictates that the solution of Eq. (4.6) does

not include the negative (positive) energy states. This observation highlights the second critical property in this kind of problems that has to be considered carefully when presenting the physical interpretation. It associates with each choice of potential configuration one sector of the energy spectrum, only the positive or the negative, but not both. This unsymmetrical treatment of the energy spectrum, where half of the spectrum is missing, is known to create problems such as particle-antiparticle interpretation of the relativistic theory [30, 44]. As for the K-G equation (4.4), we obtain the following, for $S = \pm V$

$$\left\{\vec{\nabla}^2 - 2(\varepsilon \pm m)V(\vec{r}) + \varepsilon^2 - m^2\right\}\psi_{KG}(\vec{r}) = 0 \tag{4.7}$$

which is identical to Eq. (4.6) for $\psi_{\pm}$. Nonetheless, physically this equation describes a scalar particle (spin 0) whereas Eq. (4.6) describes a spinor particle (spin $\frac{1}{2}$). However, mathematically this equivalence of the Dirac representation to the K-G representation in the presence of an interaction constitutes a constraint on the physical interpretation [44]. Moreover, the non-relativistic limit, which is obtained by taking $\varepsilon - m \cong E$ where $|E| << m$, implies that the negative energy solutions (corresponding to $S = -V$) are free fields since under these conditions Eq. (4.6) and Eq. (4.7) reduce to

$$\left(\frac{1}{2m}\vec{\nabla}^2 + E\right)\psi(\vec{r}) = 0 \tag{4.8}$$

where E is the non-relativistic energy and ψ stands for ψ_{-} or ψ_{KG}. On the other hand, the positive energy states (where $S = +V$) in the non-relativistic limit are solutions of

$$\left(\frac{1}{2m}\vec{\nabla}^2 - 2V(\vec{r}) + E\right)\psi(\vec{r}) = 0 \tag{4.9}$$

where ψ stands for ψ_+ or ψ_{KG}. This is the Schrödinger equation for the potential $2V$. Thus, we conclude that only the choice $S = +V$ produces a nontrivial non-relativistic limit with a potential function $2V$, and not V. Accordingly, it would be natural to scale the potential terms in Eq. (4.3) and Eq. (4.4) so that in the non-relativistic limit the interaction potential becomes V, not $2V$. Therefore, we modify Eq. (4.3) and Eq. (4.4) to read as follows:

$$\begin{pmatrix} m + \dfrac{V(\vec{r}) + S(\vec{r})}{2} & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -m + \dfrac{V(\vec{r}) - S(\vec{r})}{2} \end{pmatrix} \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} \tag{4.10}$$

$$\left\{\vec{\nabla}^2 + \left[\frac{1}{2}V(\vec{r}) - \varepsilon\right]^2 - \left[\frac{1}{2}S(\vec{r}) + m\right]^2\right\}\psi_{KG}(\vec{r}) = 0 \tag{4.11}$$

Consequently, Eqs. (4.6), (4.7) and (4.9) become

$$\left\{\vec{\nabla}^2 - (\varepsilon \pm m)V(\vec{r}) + \varepsilon^2 - m^2\right\}\psi_{\pm}(\vec{r}) = 0 \tag{4.12}$$

$$\left\{\vec{\nabla}^2 - (\varepsilon \pm m)V(\vec{r}) + \varepsilon^2 - m^2\right\}\psi_{KG}(\vec{r}) = 0 \tag{4.13}$$

$$\left(\frac{1}{2m}\vec{\nabla}^2 - V(\vec{r}) + E\right)\psi(\vec{r}) = 0 \tag{4.14}$$

respectively. Now it is not possible to make any further general statements beyond the three observations made above: (i) the singular matrix structure of the potential, (ii) the un-symmetrical treatment of the positive and negative energy spectrum, and (iii) the un-

favorable equivalence of the Dirac equation (4.6) to the K-G equation (4.7) in the presence of interaction. Therefore, an alternative investigation strategy based on "demonstration by example" is adopted. In other words, several choices of potential functions $V(\vec{r})$ that have well established relativistic extensions (e.g., the Dirac-Coulomb problem for which $V \propto \frac{1}{r}$) are chosen and their positive energy solutions are compared with those obtained from Eq. (4.12) or, equivalently, Eq. (4.13) for $S = +V$. The case $S = -V$ is not pursued since its non-relativistic limit is the trivial interaction-free mode. This, of course, does not diminish the importance of such problems. It only limits its contribution (with the proper physical interpretation) to the relativistic regime.

Equation (4.12) for ψ_+ and Eq. (4.13) for ψ_{KG} with $S = +V$ and for a general non-central potential $V(r,\theta,\varphi)$ could be written in spherical coordinates as follows

$$\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2}\left[(1-x^2)\frac{\partial^2}{\partial x^2}-2x\frac{\partial}{\partial x}+\frac{1}{1-x^2}\frac{\partial^2}{\partial\varphi^2}\right]-(\varepsilon+m)V+\varepsilon^2-m^2\right\}\psi=0 \quad (4.15)$$

where $x=\cos\theta$ and ψ stands for either ψ_+ or ψ_{KG}. Consequently, this equation is completely separable for potentials of the form

$$V(\vec{r}) = V_r(r)+\frac{1}{r^2}\left[V_\theta(x)+\frac{1}{1-x^2}V_\phi(\varphi)\right] \quad (4.16)$$

This is so because if we write the total wave function as $\psi(r,\theta,\varphi) = r^{-1}R(r)\Theta(\theta)\Phi(\varphi)$, then the wave equation (4.15) with the potential (4.16) gets completely separated in all three coordinates as follows

$$\left[\frac{d^2}{d\varphi^2}-(\varepsilon+m)V_\phi+E_\phi\right]\Phi=0 \tag{4.17}$$

$$\left[(1-x^2)\frac{d^2}{dx^2}-2x\frac{d}{dx}-\frac{E_\phi}{1-x^2}-(\varepsilon+m)V_\theta+E_\theta\right]\Theta=0 \tag{4.18}$$

$$\left[\frac{d^2}{dr^2}-\frac{E_\theta}{r^2}-(\varepsilon+m)V_r+\varepsilon^2-m^2\right]R=0 \tag{4.19}$$

where E_ϕ and E_θ are the separation constants, which are real and dimensionless. The components of the wave function are required to satisfy the boundary conditions. That is, $R(0)=R(\infty)=0$, $\Phi(\varphi)=\Phi(\varphi+2\pi)$, $\Theta(0)$ and $\Theta(\pi)$ are finite. Specializing to the case where $V_\phi=0$, the normalized solution of Eq. (4.17) that satisfies the boundary conditions is

$$\Phi(\varphi)=\frac{1}{\sqrt{2\pi}}e^{is\varphi},\ s\in Z=0,\pm1,\pm2,... \tag{4.20}$$

giving $E_\phi=s^2$.

The solution of Eq. (4.18) for bound states will be spanned by L^2 functions that are defined in the compact space with coordinate $x\in[-1,+1]$. Comparing it to the differential equation of the Jacobi polynomial $P_n^{(\mu,\nu)}(x)$ [45], which is also defined in the same space, we could suggest the following form of solution

$$\Theta(\theta)=A(1-x)^\alpha(1+x)^\beta P_n^{(\mu,\nu)}(x) \tag{4.21}$$

where A is the normalization constant. The real dimensionless parameters μ and ν are such that $\mu > -1$ and $\nu > -1$. Square integrability and the boundary conditions require that $\alpha > 0$ and $\beta > 0$. Substituting (4.21) into Eq. (4.18) and using the differential equation of the Jacobi polynomials we obtain

$$\left\{[\mu-\nu-2\alpha+2\beta+x(\mu+\nu-2\alpha-2\beta)]\frac{d}{dx}+2x\left(\frac{\alpha}{1-x}-\frac{\beta}{1+x}\right)+\alpha(\alpha-1)\frac{1+x}{1-x}\right.$$
$$\left.\beta(\beta-1)\frac{1-x}{1+x}-\frac{E_\phi}{1-x^2}-(\varepsilon+m)V_\theta+E_\theta-2\alpha\beta-n(n+\mu+\nu+1)\right\}P_n^{(\mu,\nu)}(x)=0 \tag{4.22}$$

Requiring that the representation in the solution space, which is spanned by (4.21), be orthogonal dictates that the x-dependent factors multiplying $P_n^{(\mu,\nu)}$ and $\frac{d}{dx}P_n^{(\mu,\nu)}$ in Eq. (4.22) must vanish. Thus, the angular potential function $V_\theta(x)$ should be of the following form

$$V_\theta(x)=\frac{a+bx}{1-x^2} \tag{4.23}$$

where a and b are real parameters. Additionally, simple manipulations of Eq. (4.22) with this potential function give the following results:

$$\mu=\sqrt{s^2+(\varepsilon+m)(a+b)} \tag{4.24}$$

$$\nu=\sqrt{s^2+(\varepsilon+m)(a-b)} \tag{4.25}$$

$$\alpha=\frac{\mu}{2},\quad \beta=\frac{\nu}{2} \tag{4.26}$$

$$E_\theta = (n+\alpha+\beta+\frac{1}{2})^2 - \frac{1}{4} \tag{4.27}$$

The Aharonov-Bohm [46] and Hartmann [41] potentials are special cases of (4.23) for which $b = 0$. For the pure Aharonov-Bohm effect, a is discrete via its linear dependence on the integer s. On the other hand, for the Hartmann problem the angular potential (4.23) should be supplemented by the radial Coulomb potential. The case where $b = \pm a$ corresponds to the magnetic monopole potential with singularity along the $\pm z$ axis [47]. The orthogonally relation of the Jacobi polynomials gives the following expression for the normalization constant that makes the angular wave functions $\{\Theta_n(\theta)\}$ an orthonormal set

$$A = \sqrt{\frac{2n+\mu+\nu+1}{2^{\mu+\nu+1}} \frac{\Gamma(n+1)\Gamma(n+\mu+\nu+1)}{\Gamma(n+\mu+1)\Gamma(n+\nu+1)}} \tag{4.28}$$

Equation (4.27) implies that for real representations we can always write $E_\theta = \lambda(\lambda+1)$, where λ is a real number, not necessarily an integer but discrete (i.e., numerable). Additionally, λ is evaluated as

$$\lambda = \begin{cases} n+\alpha+\beta & ,\lambda > 0 \\ -(n+\alpha+\beta)-1 & ,\lambda < -1 \end{cases} \tag{4.29}$$

However, real representations require that the expressions under the two square roots in Eq. (4.24) and Eq. (4.25) are non-negative. In other words, the absolute value of the integer s should be not less than some positive integer M, where M is the minimum integer that satisfies the following

$$M^2 \geq (\varepsilon + m)(|b| - a) \tag{4.30}$$

with the assumption of positive energy, corresponding to $S = +V$. Thus, the range of the integer s becomes $s = \pm M, \pm(M+1), \pm(M+2), \ldots$ and $M = 0$ only if $a \geq |b|$. For a given integer s in this range and for a given physical parameter λ, the integer n is not arbitrary but is determined by Eq. (4.29). Finally, the complete orthonormal angular wave function is given by

$$\Omega_{ns}(\theta, \varphi) = \sqrt{\frac{2n+\mu+\nu+1}{4\pi \times 2^{\mu+\nu}} \frac{\Gamma(n+1)\Gamma(n+\mu+\nu+1}{\Gamma(n+\mu+1)\Gamma(n+\nu+1)}} (1-x)^{\frac{\mu}{2}} (1+x)^{\frac{\nu}{2}} P_n^{(\mu,\nu)}(x) e^{is\varphi} \tag{4.31}$$

where the dependence on s comes also from the parameters μ and ν as given by Eq. (4.24) and Eq. (4.25), respectively.

In the following section, the radial equation will be solved to obtain the energy spectra for several radial potential functions, $V_r(r)$. These will be compared with the spectra of other closely related problems in order to make general conclusions about the validity of the interpretation of the solutions obtained for $S = \pm V$.

4.1.2. Solution of the Radial Equation and Energy Spectra for Several Examples

In the configuration space with a real coordinate *y* the wave function for bound states could be expanded in an L^2 basis $\{\chi_n\}_{n=0}^{\infty}$ as $\sum_{n=0}^{\infty} f_n(\varepsilon)\chi_n(y)$, where the basis functions

could generally be written as

$$\chi_n(y) = A_n w_n(y) P_n(y) \tag{4.32}$$

A_n is a normalization constant, $P_n(y)$ is a polynomial of degree n in y, and the weight function satisfies $w_n(y_\pm) = 0$, where $y_-(y_+)$ is the left (right) boundary of configuration space. There are two types of space that are relevant to the current problem. One for which $y_\pm$ are finite, and

$$w_n(y) = (y_+ - y)^\alpha (y - y_-)^\beta, \; P_n(y) = {}_2F_1(-n, b, c, y). \tag{4.33}$$

Another is semi-infinite where y_- finite, y_+ infinite, and therefore:

$$w_n(y) = (y - y_-)^\alpha e^{-\beta(y-y_-)}, P_n(y) = {}_1F_1(-n, c, y) \tag{4.34}$$

${}_2F_1$ is the hypergeometric function and ${}_1F_1$ is the confluent hypergeometric function [45]. The parameters α, β, a and b are real with α and β positive. They are related to the physical parameters of the problem and may depend (for bound states) on the index n. An example of the first case (4.33) is the angular wave function given in the previous section by Eq. (4.21) for which $y_\pm = \pm a$ and $P_n(y)$ are the Jacobi polynomials. On the other hand, the solution of the radial equation, Eq. (4.19), for bound states will be spanned by L^2 functions defined on the positive real line with coordinate $y \in \Re^+$, where y is proportional to some power of r. That is, the relevant configuration space is semi-infinite with $y_- = 0$. Thus, the following ansatz is compatible with this requirement and can be made to satisfy the boundary conditions

$$R(r) = By^{\tau} e^{-\xi y}\, {}_1F_1(p, q, y) \tag{4.35}$$

where B is the normalization constant, p and q are dimensionless real parameters. Square integrability and the boundary conditions require that the real dimensionless parameters τ and ξ be positive. Two cases will be considered. One, in which $y = \rho r$ and in the other $y = (\rho r)^2$, where ρ is a positive real parameter having dimension of inverse length. Substituting (4.35) into Eq. (4.19) for $y = \rho r$, $E_\theta = \lambda(\lambda+1)$, and using the differential equation of the confluent hypergeometric series, it is found:

$$\left[\left(1 - 2\xi + \frac{2\tau - q}{y}\right)\frac{d}{dy} + \frac{\tau(\tau-1) - \lambda(\lambda+1)}{y^2} + \frac{p - 2\tau\xi}{y} - \frac{\varepsilon + m}{\rho^2}V_r + \xi^2 + \frac{\varepsilon^2 - m^2}{\rho^2}\right]{}_1F_1 = 0 \tag{4.36}$$

Requiring an orthogonal representation for the bound states dictates that the y-dependent factors multiplying ${}_1F_1$ and $\frac{d}{dy}{}_1F_1(p, q, y)$ in Eq. (4.36) must independently vanish. Consequently, the radial potential function should be proportional to $\frac{1}{r}$. That is, $V_r(r) = \frac{Z}{r}$, the Coulomb potential, where Z is the charge coupling parameter which is proportional to the product of the charge number and the fine structure constant. It is worth noting that the radial potential function could also include a term proportional to r^{-2} without destroying the solvability of Eq. (4.36). However, by a redefinition of the separation constant E_θ in Eq. (4.19), such a term could easily be absorbed into the

centripetal potential E_θ / r^2. Now, for bound states $Z < 0$ and the confluent hypergeometric series ${}_1F_1(p, q, y)$ must terminate which requires that $p = -k$, where $k = 0,1,2,...$. Simple manipulations of Eq. (4.36) give the following results:

$$\tau = n + \alpha + \beta + 1,\ \xi = \frac{1}{2},\ q = 2\tau \tag{4.37}$$

$$\varepsilon_{kns} = m\frac{(k + n + \alpha + \beta + 1)^2 - Z^2/4}{(k + n + \alpha + \beta + 1)^2 + Z^2/4} \tag{4.38}$$

$$\rho = -Z\frac{\varepsilon_{kns} + m}{k + n + \alpha + \beta + 1} \tag{4.39}$$

The dependence of the energy spectrum on the integer s comes from the parameters α and β as given by Eqs. (4.24-26). Moreover, it is obvious that the upper bound of this positive energy spectrum ($\varepsilon = +m$) is obtained for large values of quanta k and/or n. Of course, the negative energy spectrum and its lower bound ($\varepsilon = -m$) is obtained by considering the case $S = -V$. If this formulation of the relativistic problem is misinterpreted, one may presume that the energy spectrum (4.38) includes that of the relativistic Coulomb problem (when $a = b = 0$) and that of the relativistic Hartmann problem (when $a \neq 0$ and $b = 0$). Obviously, the spectra of other problems (e.g., the magnetic monopole where $Z = 0$ and $b = \pm a$) could also be assumed incorrectly to be included, but will not be discussed here. For the Coulomb case, $\alpha = \beta = \frac{|s|}{2}$ and the energy spectrum (4.38) is written as

$$\varepsilon_{kl} = m\frac{(k+l+1)^2 - Z^2/4}{(k+l+1)^2 + Z^2/4} \tag{4.40}$$

where $l = n + |s| = 0, 1, 2, \ldots$. This is not equal to the well-known positive energy spectrum of the relativistic Dirac-Coulomb problem (see Sec.3.3.4),

$$\varepsilon_{kl} = m\left[1 + \frac{Z^2}{\left(k + \sqrt{(l+1)^2 - Z^2}\right)^2}\right]^{-1/2} \tag{4.41}$$

However, both give the correct non-relativistic limit (in the case of weak coupling, i.e. $Z << 1$ and $|E| << m$):

$$E_{kl} = -\frac{mZ^2}{2(k+l+1)^2} \tag{4.42}$$

As for the Hartmann problem, it is well known that taking the limit $a \to 0$ gives the Coulomb problem. Therefore, we can also conclude that the correct relativistic extension of the Hartmann problem is not as formulated above [42]. Nevertheless, the non-relativistic limit ($Z << 1$) of the energy spectrum (4.38) for the Hartmann problem, where $a \neq 0$, $b = 0$ and $\alpha = \beta = \frac{1}{2}\sqrt{s^2 + a(\varepsilon + m)}$, is

$$E_{kns} = -\frac{mZ^2}{2}\left(k + n + 1 + \sqrt{s^2 + 2ma}\right)^{-2} \tag{4.43}$$

which is the correct non-relativistic spectrum [41,48].

Taking $y=(\rho r)^2$ in the radial wave function (4.35) and employing the differential equation of the confluent hypergeometric series reduce Eq. (4.19) to the following

$$\left[\left(1-2\xi+\frac{2\tau-q+\frac{1}{2}}{y}\right)y\frac{d}{dy}+\frac{2\tau(2\tau-1)-\lambda(\lambda+1)}{4y}+\xi^2 y-\frac{\varepsilon+m}{4\rho^2}V_r+p-\xi\left(2\tau+\frac{1}{2}\right)+\frac{\varepsilon^2-m^2}{4\rho^2}\right]{}_1F_1=0 \tag{4.44}$$

Orthogonal representation for the bound states dictates that the factors multiplying ${}_1F_1$ and $\frac{d}{dy}{}_1F_1(p,q,y)$ must vanish. Thus, the radial potential function should be proportional to r^2. That is, we can write $V_r(r)=\frac{1}{2}m\omega^2 r^2$, which is the potential for the 3D isotropic oscillator with ω being the oscillator frequency. Similarly to the Coulomb problem, this radial potential could also include a term proportional to y^{-1} (i.e., r^{-2}). Such a term could be absorbed, as well, into the centripetal potential E_θ / r^2. For bound states the confluent hypergeometric series must terminate, requiring that $p=-k$, where $k=0,1,2,...$. Simple manipulations of Eq. (4.44) give the following results:

$$2\tau=n+\alpha+\beta+1,\ \xi=\frac{1}{2},\ q=2\tau+\frac{1}{2} \tag{4.45}$$

$$(\varepsilon_{kns}-m)\sqrt{\frac{\varepsilon_{kns}+m}{2m}}=\omega\left(2k+n+\alpha+\beta+\frac{3}{2}\right) \tag{4.46}$$

$$\rho^4 = \frac{1}{2} m\omega^2 (\varepsilon_{kns} + m) \tag{4.47}$$

The relativistic bound state energy spectrum is obtained by solving Eq. (4.46) for ε_{kns}.

For the spherically symmetric case, where $a = b = 0$ and $\alpha = \beta = \frac{|s|}{2}$, the right hand side of Eq. (4.46) becomes $\omega\left(2k + l + \frac{3}{2}\right)$. The resulting formula will be compared to the well-known positive energy spectrum of the Dirac-oscillator (see Section 3.3.5):

$$\varepsilon_{kl} = m\begin{cases} \sqrt{1+4\frac{\omega}{m}\left(k+l+\frac{3}{2}\right)}, & \ell = \mathrm{j}+\frac{1}{2} \\ \sqrt{1+4\frac{\omega}{m}k}\,, & \ell = \mathrm{j}-\frac{1}{2} \end{cases} \tag{4.48}$$

where j is the total angular momentum, orbital plus spin. It is obvious that the two relativistic spectra do not coincide. Nevertheless, the non-relativistic limit (when $|E| << m$ and $\omega << m$) of Eq. (4.46), which describes the oscillator in the presence of the non-central potential (4.23), is

$$E_{kns} = \omega\left(2k + n + \alpha + \beta + \frac{3}{2}\right) \tag{4.49}$$

which is the correct spectrum [12,47].

The three examples presented above (the Coulomb, Hartmann, and oscillator) show that the formulation of the relativistic problem, as depicted in Eqs. (4.3-4) [equivalently, Eqs. (4.10-11)] with $S = +V$, should not be misinterpreted as equivalent to those that

have the same non-relativistic limit. This is compatible with the view that although the non-relativistic limit is well defined and unique, the relativistic extension is not.

4.2. The Klein-Gordon Equation with Unequal Scalar and Vector Potentials

For the sake of completeness, in this section, I will study a related problem that has received as much attention as the subject of Section 4.1 [49]. It deals with the K-G equation (4.4) [equivalently, Eq. (4.11)] but with unbalanced potential contributions in which $S = \eta V$, where η is a real parameter such that $\eta \neq \pm 1$. This case does not suffer from the singular potential structure mentioned below Eq. (4.4). Additionally, the Dirac and K-G equations give results that are equivalent *only* under certain physical constraints. Thus, fruitful results are expected. As an illustrative example, spherically symmetric exponential-type potentials leading to the correct formulation of the relativistic extension of the S-wave Morse problem will be studied [50]. It bears a very close resemblance to the Dirac-Morse problem [2].

The radial component of the K-G equation (4.11) for spherically symmetric potentials, with $S = \eta V$ and $V(r) = V_0 e^{-\rho r}$, reads as follows

$$\left[\frac{d^2}{dr^2} - \frac{1}{4}\left(\eta^2 - 1\right)V_0^2 e^{-2\rho r} - (\varepsilon + \eta m)V_0 e^{-\rho r} + \varepsilon^2 - m^2\right]R(r) = 0 \tag{4.50}$$

where V_0 and ρ are real potential parameters and ρ positive. On the other hand, the Dirac-Morse potential [2] is a three-parameter relativistic extension of the S-wave Morse

oscillator. The "kinetic balance" relation in that problem could be used to eliminate the lower spinor component giving the following second order radial differential equation [2] for the upper component

$$\left[\frac{d^2}{dr^2}-(A_0/\zeta)^2 e^{-2\rho r}-(2\varepsilon+\frac{\rho}{\zeta})A_0 e^{-\rho r}+\varepsilon^2-m^2\right]R(r)=0 \tag{4.51}$$

where $\{\zeta,\rho,A_0\}$ are the physical parameters of the problem such that, for bound states, $\zeta^2=(2A_0/\rho)^2$. Comparing this equation with Eq. (4.50) shows that the current K-G problem is an S-wave Dirac-Morse problem if $A_0=\frac{1}{2}V_0$, $\zeta=\frac{1}{2}(\rho/\eta m)$ and only for the restricted case where $\zeta^2=(\rho/2m)^2-1$ and $\rho>2m$ (i.e., only if $\eta^2=[1-(2m/\rho)^2]^{-1}$). To pursue the solution of the current K-G problem, assume the following radial wave function which is compatible with the domain of the wave operator (4.50)

$$R(r)=Az^{\tau}e^{-\xi z}{}_1F_1(p,q,z) \tag{4.52}$$

where $z=e^{-\rho r}$ and, for economy of notation, use was made of the same symbols as those in the previous section. Substituting this in Eq. (4.50) and using the differential equation of the confluent hypergeometric series, the following is found

$$\left[\left(1-2\xi+\frac{2\tau-q+1}{z}\right)\frac{d}{dz}+\frac{\tau^2+(\varepsilon^2-m^2)/\rho^2}{y^2}-\frac{\eta^2-1}{4\rho^2}V_0^2+\xi^2 -\frac{\xi(2\tau+1)-p+V_0(\varepsilon+\eta m)/\rho^2}{z}\right]{}_1F_1=0 \tag{4.53}$$

to obtain real solutions of this equation, I require that $\eta V_0 < 0$. For bound states $p = -n$, where $n = 0, 1, 2, ...$. Moreover, the wave function parameters are evaluated as follows

$$\tau = \chi - n - \frac{1}{2} - \left(V_0 / \rho^2\right)\varepsilon_n, \quad \xi = \frac{1}{2} \tag{4.54}$$

$$q = 2\tau + 1, \quad \eta^2 = 1 + \left(\rho / V_0\right)^2 \tag{4.55}$$

and the relativistic energy spectrum is derived as

$$\left[1 + (V_0 / \rho)^2\right]\varepsilon_n = V_0\left(\chi - n - \frac{1}{2}\right) \pm \rho\sqrt{\left(n + \frac{1}{2}\right)\left(2\chi - n - \frac{1}{2}\right)} \tag{4.56}$$

where $\chi = \frac{m}{\rho}\sqrt{1 + \left(V_0 / \rho\right)^2}$ and $n \le 2\chi - \frac{1}{2}$. These results show that the Klein-Gordon-Morse problem is equivalent to the Dirac-Morse problem if and only if the potential parameters are related as $V_0^2 = \rho^2\left[(\rho / 2m)^2 - 1\right]$.

4.3. The Dirac Equation with Spin and Pseudo-Spin Symmetry

Similar to problems treated above are those with what is called spin and pseudo-spin symmetries. These are widely used in nuclear physics to account for discrepancies in some of the non-relativistic spectrum calculations [14]. In these studies, the Dirac equation is coupled , as in the case of equal scalar-vector method, to a scalar (S) and a four-vector with vanishing space-like components leaving the field (V) but here the relation between these two fields is taken as $S = C_s + V$ for spin symmetry and

$S = C_{ps} - V$ for pseudo-spin symmetry where C_s and C_{ps} are constants. Usually these constants are taken to represent an attractive mean field where nucleons (inside a nucleus) move independently. The vector field is taken to be repulsive. Rewriting Eq. (4.3):

$$\begin{pmatrix} m + S(\vec{r}) + V(\vec{r}) & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -m - S(\vec{r}) + V(\vec{r}) \end{pmatrix} \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}, \tag{4.3}$$

Now making the substitution $S = \eta \pm V$ (where η is either C_s or C_{ps}) leads to:

$$\begin{pmatrix} m + \eta \pm V(\vec{r}) + V(\vec{r}) & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -m - \eta \mp V(\vec{r}) + V(\vec{r}) \end{pmatrix} \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}, \tag{4.57}$$

Therefore, for spin symmetry Eq. (4.57) reads

$$\begin{pmatrix} (m + C_s) + 2V(\vec{r}) & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -(m + C_s) \end{pmatrix} \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}, \tag{4.58}$$

While for pseudo-spin symmetry, Eq. 4.57 reads

$$\begin{pmatrix} (m + C_{ps}) & -i\vec{\sigma}\cdot\vec{\nabla} \\ -i\vec{\sigma}\cdot\vec{\nabla} & -(m + C_{ps}) + 2V(\vec{r}) \end{pmatrix} \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}, \tag{4.59}$$

Comparing these two equations with Eq. (4.3), with $S = \pm V$, shows that the spin symmetry case is the same as $S = +V$ but with the mass m replaced by $m + C_s$. On the other hand, the pseudo-spin symmetry is the same as the case $S = -V$ but with the mass m replaced by $m + C_{ps}$. Therefore, all the solutions found in Section 4.1 can be used in the current problem after the replacement of the mass as discussed above. Notice that

these solutions in the domain of nuclear studies are not criticized as is the case in Section 4.1 because their physical interpretation is well founded.

CHAPTER 5

THE NON-RELATIVISTIC LIMIT OF THE DIRAC EQUATION WITH SPATIALLY DEPENDENT EFFECTIVE MASS

5.1. The Role of Position Dependent Mass in Physics

Calculations of physical quantities relevant to semiconductors are sometimes done using the effective mass approximation. Initially this approximation was used to describe impurities in crystals where much of the interaction with the host lattice is parameterized through an effective mass parameter in the impurity Hamiltonian [51]. The effective mass is also an important parameter in Landau's Fermi liquid theory that deals with low-level excited states of strongly interacting systems in a very appealing single particle approximation. Since then, the effective mass approximation has become an essential ingredient in describing the transport properties of semi-conductor hetero-junctions and quantum dots [15]. One of the main features of these hetero-junctions or graded semiconductors is that the effective mass of the charge carriers is position dependent and frequently results from discontinuities in the effective mass across the hetero-junction with abrupt interfaces. Thus, one is lead to study quantum mechanical problems with position-dependent effective mass. However, such treatments encounter a nontrivial problem related to the ordering ambiguity in the quantization of the momentum and mass

operators in the kinetic energy term of the effective Hamiltonian.

On the other hand, relativistic effects have a significant influence on the electronic properties of materials containing heavy atoms or those that are doped with heavy ions because the charge carriers in such materials attain high velocities comparable to that of light. Relativistic effects also include spin-orbit and spin-spin couplings that are purely relativistic corrections to the non-relativistic Hamiltonians. The Spin-orbit interaction, in particular, alters the spectroscopic properties of molecules containing heavy elements to a considerable extent. Thus, the solution of the Dirac equation under the circumstance where the mass depends on the position of electrons will be of interest in studying materials containing heavy elements.

The quantization of non-relativistic Hamiltonians of position-dependent mass systems is always hindered by ordering ambiguities in the kinetic energy term. On the other hand its relativistic counterpart, the relativistic Dirac equation, does not suffer from such an ambiguity. This ordering ambiguity of mass and momentum is due to the fact that these two quantities no longer commute when the mass is space dependent. An effective approach towards the resolution of this ambiguity is to start with the relativistic Dirac wave equation which does not suffer from any ordering problem, then take the non-relativistic limit which is well defined and unique. Of course, the full Dirac equation can be used in problems with position dependent mass. However, knowing the extreme difficulties in finding non-trivial solutions of Dirac equations with fixed mass (let alone with varying mass) as seen in Chapter 3, makes this approach impractical. In reality,

solutions of Dirac equation with position dependent mass are scarce [9]. There have been several attempts in defining the correct Hermitian kinetic energy operator for a variable mass system based on current conservation [15], Galilean invariance [52] or the recent supersymmetric treatment of the effective mass Hamiltonians [53]. It is believed that the work of Cavalcante et al. [16] is a measurable contribution towards the resolution of the ordering ambiguity problem of the quantum kinetic-energy operator with spatially varying effective mass. In their work, the non-relativistic limit of the Dirac equation was calculated using the technique of the Foldy-Wouthuysen Transformation.

In this chapter, the same procedure will be followed but more systematically. At first, I will reproduce their results concerning the kinetic operator. Secondly, a new term they missed will also be derived. Finally the non-relativistic Hamiltonian up the fourth order in the Compton wavelength will be calculated.

5.2. Review of Foldy-Wouthuysen Transformation

Given a Dirac Hamiltonian H (free Hamiltonian plus potential coupling), then a Fouldy-Wouthuysen transformation (FWT) is a unitary operator

$$FWT = e^{i\hat{S}(\vec{r})} \tag{5.1}$$

that gives a new wave function (spinor) and Hamiltonian as follows:

$$\psi(\vec{r},t)' = e^{i\hat{S}(\vec{r})}\,\psi(\vec{r},t) \tag{5.2}$$

$$H' = e^{iS(\vec{r})} H e^{-iS(\vec{r})} = H + i[S,H] + \frac{i^2}{2!}[S,[S,H]] + \frac{i^3}{3!}[S,[S,[S,H]]] + \cdots \tag{5.3}$$

Where only time-independent transformations are treated [29-30, 35, 54]. The aim of FWT is to choose S such that odd operators in the Hamiltonian are absent in the expansion (5.3) up to a chosen order in c^{-2}. That is, the upper and lower components of the Dirac spinor decouple for that order of c^{-2}. To make this clear, notice that a spinor (with its four components) can be written in terms of two-components spinors as

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \begin{bmatrix} \psi_+ \\ \psi_- \end{bmatrix}, \text{ where } \psi_+ = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \text{ and } \psi_- = \begin{bmatrix} \psi_3 \\ \psi_4 \end{bmatrix} \tag{5.4}$$

Now the Dirac Hamiltonian is a matrix (with differential elements) that can be written in terms of 2×2 matrices as

$$H = \begin{bmatrix} H11 & H12 \\ H21 & H22 \end{bmatrix} = \begin{bmatrix} H11 & 0 \\ 0 & H22 \end{bmatrix} + \begin{bmatrix} 0 & H12 \\ H21 & 0 \end{bmatrix} \tag{5.5}$$

The two terms in Eq. (5.5) are called even and odd operators, respectively. In the Dirac equation, even operators do not mix the two components of the spinor $(\psi_{\pm})$ while the odd ones do. At the non-relativistic limit of the Dirac equation, the upper component (ψ_+) describes an electron while the other component describes an anti-electron (positron). Thus, it is required to find an equation that describes an electron (at non-relativistic energy) alone. However, the full Dirac Hamiltonian is neither even nor odd. This is why FWT is required to decouple the two spinor components. Of course, FWT

does not change the physics since it is a unitary operator. For the free Dirac Hamiltonian, it is possible to find a FWT that *completely* decouple the even operator from the odd one [29-30, 35]. Nevertheless, for an interacting particle this is generally not possible. However, at the non-relativistic limit, the odd operator is of lower order than the even one (see bellow). Thus, the hope is to choose S in Eq. (5.3) such that H' does not have an odd operator to some power of c^{-2}. Then this new Hamiltonian can be used as an approximation to our problem up to that chosen power of c^{-2}. We can then do another FWT to get to a better approximation, and so on.

5.3. The Non-Relativistic Limit of the Dirac Equation with position-dependent mass

5.3.1. Formulation of the Problem

In this work, the Hamiltonian will be a free Dirac Hamiltonian with an electromagnetic interaction [55] and position dependent mass:

$$\hat{H} = m\hat{\beta} + \lambda\hat{O} + \lambda^2 V \tag{5.6}$$

Where $\hat{O} = \hat{\alpha}\cdot\hat{\pi} = \hat{\alpha}\cdot\left(\hat{p} - \vec{A}\right)$, $(V,\ \vec{A})$ is the four vector of the electromagnetic potential, $\hat{\beta} = \begin{bmatrix} 1_{2\times2} & 0 \\ 0 & -1_{2\times2} \end{bmatrix}$ and $\hat{\alpha}$ is the matrix vector with components $\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}$ where σ_i are the Pauli matrices given by $\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ and $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. The

$1_{2\times2}$ is the 2×2 unit matrix. The only odd operator in Eq. (5.6) is $\hat{O}$. The units used in Eq. (5.6) are the atomic units $m_0 = \hbar = e = 1$, where the physical mass is given by $M(\vec{r}) = m_0 m(\vec{r})$ such that m is dimensionless. λ is the Compton wavelength given by $\frac{\hbar}{m_0 c}$ or for the chosen units $\lambda = \frac{1}{c}$. It can be seen from this that the non-relativistic limit where $c \to \infty$ is equivalent to the limit where $\lambda \to 0$. The main objective now is to use the FWT to derive the non-relativistic limit of Eq. (5.6) to fourth order in λ by requiring that the odd operator of the resulting Hamiltonian to be of the fifth or higher order in λ. Two FWT will be needed to accomplish this objective.

5.3.2. The Non-Relativistic Limit of the Dirac Equation

As mentioned above, two consecutive FWTs will be applied to the Hamiltonian in Eq. (5.6). The first FWT is chosen to be of the form:

$$\hat{S} = \lambda\hat{\eta} = -\frac{\lambda}{2im}\hat{O}\hat{\beta} + \frac{\lambda}{4im^2}(\hat{\alpha}\cdot\hat{p}m)\hat{\beta} \tag{5.7}$$

where the operator $\hat{\eta}$ is defined by this equation. Then it can be shown that

$$\hat{O} + i\left[\hat{\eta}, m\hat{\beta}\right] = 0 \Rightarrow \left[\hat{\eta}, m\hat{\beta}\right] = i\hat{O} \tag{5.8}$$

Applying this to Eq. (5.3) leads to the following Hamiltonian to the order λ^4

$$H' = m\hat{\beta} + \lambda^2 V + i\lambda^2\left[\hat{\eta}, \hat{O}\right] + i\lambda^3[\eta, V] + \frac{i^2\lambda^2}{2!}\left[\hat{\eta}, \left[\hat{\eta}, m\hat{\beta}\right]\right] + \frac{i^2\lambda^3}{2!}\left[\hat{\eta}, \left[\hat{\eta}, \hat{O}\right]\right]$$
$$-\frac{\lambda^4}{2!}[\hat{\eta}, [\hat{\eta}, V]] + \frac{i^3\lambda^3}{3!}\left[\hat{\eta}, \left[\hat{\eta}, \left[\hat{\eta}, m\hat{\beta}\right]\right]\right] + \frac{i^3\lambda^4}{3!}\left[\hat{\eta}, \left[\hat{\eta}, \left[\hat{\eta}, \hat{O}\right]\right]\right] + \frac{i^4\lambda^4}{4!}\left[\hat{\eta}, \left[\hat{\eta}, \left[\hat{\eta}, \left[\hat{\eta}, m\hat{\beta}\right]\right]\right]\right] \quad (5.9)$$

Thus, the odd operator is cancelled to order λ^2. Using Eq. (5.8) again and rearranging leads to:

$$H' = m\hat{\beta} + \lambda^2 V + i\frac{\lambda^2}{2}\left[\hat{\eta}, \hat{O}\right] - \frac{\lambda^4}{2}[\hat{\eta}, [\hat{\eta}, V]] - \frac{i\lambda^4}{8}\left[\hat{\eta}, \left[\hat{\eta}, \left[\hat{\eta}, \hat{O}\right]\right]\right] + \lambda^3(odd - terms) \quad (5.10)$$

The odd terms were not written because they will be eliminated and thus not needed explicitly. The remaining odd operator will now be cancelled by a second FWT.

Now a second FWT is chosen in the form:

$$\hat{S} = \lambda^3\hat{\rho} \quad (5.11)$$

The new Hamiltonian H'' is then, according to Eq. (5.3):

$$H'' = H' + i\lambda^3[\rho, H'] + O(\lambda^6) \Rightarrow H'' = H' + i\lambda^3\left[\rho, m\hat{\beta}\right] + O\left(\lambda^5\right) \quad (5.12)$$

Now ρ can be chosen to cancel the remaining odd terms in H' leading to the final Hamiltonian

$$H'' = m\hat{\beta} + \lambda^2 V + i\frac{\lambda^2}{2}\left[\eta, \hat{O}\right] - \frac{\lambda^4}{2}[\eta, [\eta, V]] - \frac{i\lambda^4}{8}\left[\eta, \left[\eta, \left[\eta, \hat{O}\right]\right]\right] \quad (5.13)$$

Notice that there is no need to write the explicit form of ρ and it is enough to snow that it exists. Physically it is known that the non-relativistic limit exists which is enough to

prove on physical grounds the existence of $\hat{\rho}$. The commutators in (5.13) are given by

(where $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$):

$$\frac{i\lambda}{2}\left[\hat{\eta}, \hat{O}\right] = \frac{\lambda^2}{2m}\hat{\pi}^2\hat{\beta} - \frac{i\lambda^2}{2m}\hat{\Sigma}\cdot\left(\vec{p}\times\vec{A}\right)\hat{\beta} - \frac{\lambda^2}{2m^2}(\vec{p}m)\cdot\hat{\pi}\beta - \frac{i\lambda^2}{4m^2}\hat{\Sigma}\cdot(\vec{p}m)\times\hat{\pi}\hat{\beta}$$
$$-\frac{\lambda^2}{8m^2}\left(\vec{p}^{\,2}m\right)\hat{\beta} + \frac{\lambda^2}{4m^3}(\vec{p}m)^2\hat{\beta} \tag{5.14}$$

$$-\frac{\lambda^4}{2}[\hat{\eta},[\hat{\eta},V]] = -\frac{\lambda^4}{8m^2}\left(\vec{p}^{\,2}V\right) + \frac{i\lambda^4}{4m^2}\hat{\Sigma}\cdot(\vec{p}V)\times\hat{\pi} + \frac{\lambda^4}{8m^3}(\vec{p}m)\cdot(\vec{p}V) + \frac{i\lambda^4}{4m^3}\hat{\Sigma}\cdot(\vec{p}m)\times(\vec{p}V) \tag{5.15}$$

$$-\frac{i\lambda^4}{8}\left[\hat{\eta},\left[\hat{\eta},\left[\hat{\eta},\hat{O}\right]\right]\right]=-\frac{\lambda^4}{8m^3}\,p^4\beta+\frac{3\lambda^4}{4m^4}(pm)\cdot pp^2\beta-\frac{7\lambda^4}{32im^4}\Sigma\cdot(pm)\times pp^2\beta-\frac{13\lambda^4}{16m^5}(pm)^2\,p^2\beta$$
$$+\frac{5\lambda^4}{16m^4}\left(p^2m\right)p^2\beta-\frac{5\lambda^4}{16m^5}(\alpha\cdot pm)(pm)\cdot p\alpha\cdot p\beta+\frac{11\lambda^4}{32m^4}(\alpha\cdot ppm)\cdot p\alpha\cdot p\beta$$
$$-\frac{27\lambda^4}{32m^5}(\alpha\cdot pm)(pm)\cdot p\alpha\cdot p\beta-\frac{\lambda^4}{4m^5}(\alpha\cdot ppm)\cdot(pm)\alpha\cdot p\beta+\frac{\lambda^4}{2m^6}(\alpha\cdot pm)(pm)^2\alpha\cdot p\beta$$
$$+\frac{\lambda^4}{32im^5}(\alpha\cdot pm)\Sigma\cdot(pm)\times p\alpha\cdot p\beta-\frac{\lambda^4}{32im^4}\alpha_i\Sigma\cdot(p_i\,pm)\times p\alpha\cdot p\beta+\frac{9\lambda^4}{16m^5}(p_im)(pm)\cdot pp_i\beta$$
$$+\frac{9\lambda^4}{32m^5}(\alpha\cdot pm)(pm)\cdot p\alpha\cdot p\beta+\frac{3\lambda^4}{16m^4}(p_i\,pm)\cdot pp_i\beta-\frac{3\lambda^4}{32m^4}(\alpha\cdot ppm)\cdot p\alpha\cdot p\beta$$
$$+\frac{\lambda^4}{32im^5}\alpha_i(\alpha\cdot pm)\Sigma\cdot(pm)\times pp_i\beta-\frac{\lambda^4}{64im^4}\alpha_i\alpha_j\Sigma\cdot\left(p_j\,pm\right)\times pp_i\beta-\frac{55\lambda^4}{128m^5}(\alpha\cdot pm)\left(p^2m\right)\alpha\cdot p\beta$$
$$+\frac{53\lambda^4}{32m^6}(\alpha\cdot pm)(pm)^2\alpha\cdot p\beta-\frac{\lambda^4}{2m^5}(pm)\cdot(\alpha\cdot ppm)\alpha\cdot p\beta+\frac{\lambda^4}{8m^4}\left(\alpha\cdot pp^2m\right)\alpha\cdot p\beta$$
$$+\frac{\lambda^4}{64im^5}\alpha_i\Sigma\cdot(p_i\,pm)\times(pm)\alpha\cdot p\beta+\frac{\lambda^4}{128im^5}\Sigma\cdot(pm)\times(\alpha\cdot ppm)\alpha\cdot p\beta-\frac{7\lambda^4}{16m^5}(\alpha\cdot pm)(\alpha\cdot ppm)\cdot p\beta$$
$$+\frac{37\lambda^4}{32m^6}(pm)^2(pm)\cdot p\beta-\frac{\lambda^4}{4m^5}[(pm)\cdot ppm]\cdot p\beta-\frac{29\lambda^4}{64m^5}\left(p^2m\right)(pm)\cdot p\beta+\frac{11\lambda^4}{64m^4}\left(p^2\,pm\right)\cdot p\beta$$
$$-\frac{\lambda^4}{8m^5}\alpha_i(pm)\cdot(\alpha\cdot ppm)p_i\beta+\frac{\lambda^4}{64m^4}\alpha_i\left(\alpha\cdot pp^2m\right)p_i\beta+\frac{9\lambda^4}{32m^6}(pm)^2\alpha_i(\alpha\cdot pm)p_i\beta$$
$$-\frac{7\lambda^4}{64m^5}\left(p^2m\right)\alpha_i(\alpha\cdot pm)p_i\beta-\frac{\lambda^4}{32m^5}(\alpha\cdot pp_im)(\alpha\cdot pm)p_i\beta-\frac{7\lambda^4}{32m^5}(pm)\cdot(p_i\,pm)p_i\beta$$
$$+\frac{\lambda^4}{128im^5}\alpha_i\Sigma\cdot(pm)\times(\alpha\cdot ppm)p_i\beta+\frac{\lambda^4}{32im^5}\left(p^2m\right)\Sigma\cdot(pm)\times p\beta-\frac{9\lambda^4}{64im^6}(pm)^2\Sigma\cdot(pm)\times p\beta$$

$$+\frac{\lambda^4}{32im^5}\alpha_i(\alpha\cdot pm)\Sigma\cdot(p_i pm)\times p\beta-\frac{\lambda^4}{64im^6}(\alpha\cdot pm)(p_i m)\Sigma\cdot(pm)\alpha_i\times p\beta$$
$$+\frac{3\lambda^4}{64im^5}(\alpha\cdot pm)\alpha_i\Sigma\cdot(p_i pm)\times p\beta-\frac{\lambda^4}{64im^4}\alpha_j\alpha_i\Sigma\cdot(p_i p_j pm)\times p\beta+\frac{7\lambda^4}{128m^4}(p^4 m)\beta$$
$$+\frac{\lambda^4}{128im^5}(\alpha\cdot pm)\alpha_i\Sigma\cdot(p_i pm)\times p\beta+\frac{\lambda^4}{128im^5}(p_j m)\alpha_i\Sigma\cdot(p_i pm)\alpha_j\times p\beta-\frac{29\lambda^4}{128m^5}(\alpha\cdot pm)(\alpha\cdot pp^2 m)\beta$$
$$+\frac{65\lambda^4}{64m^6}(\alpha\cdot pm)(\alpha\cdot ppm)\cdot(pm)\beta+\frac{13\lambda^4}{16m^6}(pm)\cdot(\alpha\cdot ppm)(\alpha\cdot pm)\beta-\frac{77\lambda^4}{32m^7}(pm)^4\beta$$
$$+\frac{145\lambda^4}{16m^6}(p^2 m)(pm)^2\beta-\frac{41\lambda^4}{128m^5}(p^2 pm)\cdot(pm)\beta-\frac{\lambda^4}{8m^5}\alpha_i(\alpha\cdot ppm)\cdot(p_i pm)\beta-\frac{15\lambda^4}{128m^5}(p^2 m)^2\beta$$
$$+\frac{\lambda^4}{4m^6}(pm)\cdot[(pm)\cdot(ppm)]\beta-\frac{3\lambda^4}{128m^5}(p^2 m)^2\beta-\frac{9\lambda^4}{64m^5}(\alpha\cdot ppm)^2\beta-\frac{7\lambda^4}{128m^5}\alpha_i(\alpha\cdot pm)(p^2 p_i m)\beta$$
$$+\frac{7\lambda^4}{64m^6}(p_i m)(pm)\cdot(p_i pm)\beta-\frac{13\lambda^4}{256im^6}(\alpha\cdot pm)\Sigma\cdot(pm)\times(\alpha\cdot ppm)\beta$$
$$+\frac{\lambda^4}{64im^5}\alpha_i\Sigma\cdot(p_i pm)\times(\alpha\cdot ppm)\beta-\frac{\lambda^4}{64im^6}\alpha_i\Sigma\cdot(p_i pm)\times(pm)(\alpha\cdot pm)\beta$$
$$-\frac{\lambda^4}{128im^6}\Sigma\cdot(pm)\times(\alpha\cdot ppm)(\alpha\cdot pm)\beta+\frac{\lambda^4}{128im^5}\alpha_i\Sigma\cdot(pm)\times(\alpha\cdot pp_i pm)\beta \tag{5.16}$$

Finally summing up the terms in (5.13) leads to

$$H''=m\hat{\beta}+\lambda^2 V+\frac{\lambda^2}{2m}\pi^2\beta-\frac{i\lambda^2}{2m}\Sigma\cdot(p\times A)\beta-\frac{\lambda^2}{2m^2}(pm)\cdot\pi\beta-\frac{i\lambda^2}{4m^2}\Sigma\cdot(pm)\times\pi\beta$$
$$-\frac{\lambda^2}{8m^2}(p^2 m)\beta+\frac{\lambda^2}{4m^3}(pm)^2\beta-\frac{\lambda^4}{8m^2}(p^2 V)+\frac{i\lambda^4}{4m^2}\Sigma\cdot(pV)\times\pi+\frac{\lambda^4}{8m^3}(pm)\cdot(pV) \tag{5.17}$$
$$+\frac{i\lambda^4}{4m^3}\Sigma\cdot(pm)\times(pV)-\frac{i\lambda^4}{8}[\eta,[\eta,[\eta,O]]]+O(\lambda^5)$$

Where the last term is given by (5.16). The new Hamiltonian contains the usual terms found for constant mass plus terms proportional to the derivative of the position-dependent mass [29-30, 35]. The result of this work is that now Dirac's equation to λ^4 has the form:

$$\begin{pmatrix} H''_{11} & 0 \\ 0 & H''_{22} \end{pmatrix}\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \varepsilon\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \tag{5.18}$$

Where H_{11} and H_{22} are given by the even Hamiltonian in Eq. (5.17) and $\varepsilon \approx m + \lambda^2 \tilde{E}$.

Therefore, the two components of the spinor have separate equation as follows:

$$\left(H''_{11} - \varepsilon\right)\psi_+ = 0 \tag{5.19}$$

$$\left(H''_{22} - \varepsilon\right)\psi_- = 0 \tag{5.20}$$

This is the meaning of the non-relativistic limit where the two components of the spinor decouple.

To study the effect of the dependence of mass on position without the complications of the electromagnetic field, let the electromagnetic field vanish and keep only the second order terms. We will see that the dependence of mass on position produce effective interaction despite that the Hamiltonian is free. This is a well-known fact for such systems. In this limit, the Hamiltonian in Eq. (5.17) becomes:

$$H_0 = m\hat{\beta} + \frac{\lambda^2}{2m}\vec{p}^{\,2}\beta - \frac{\lambda^2}{2m^2}(pm)\cdot\vec{p}\beta - \frac{i\lambda^2}{4m^2}\Sigma\cdot(pm)\times\vec{p}\beta - \frac{\lambda^2}{8m^2}\left(p^2 m\right)\beta + \frac{\lambda^2}{4m^3}(pm)^2\beta \tag{5.21}$$

Where the zero index in the Hamiltonian indicates that there is no interaction. This Hamiltonian may be written as:

$$H_0 = m\beta + K + h \tag{5.22}$$

$$K = \frac{\lambda^2}{2m}\vec{p}^{\,2}\beta - \frac{\lambda^2}{2m^2}(pm)\cdot\vec{p}\beta - \frac{\lambda^2}{8m^2}\left(p^2 m\right)\beta + \frac{\lambda^2}{4m^3}(pm)^2\beta \tag{5.23}$$

$$h = \frac{i\lambda^2}{4m^2}\vec{\Sigma}\cdot(\vec{p}m)\times\vec{p}\beta \tag{5.24}$$

The first term in this Hamiltonian is naturally the rest mass contribution. The operator K is the kinetic operator. It can also be written as follows:

$$K = \frac{\lambda^2}{4}\left[\frac{1}{\sqrt{m}}\vec{p}\cdot\frac{1}{\sqrt{m}}\vec{p} + \vec{p}\cdot\frac{1}{\sqrt{m}}\vec{p}\frac{1}{\sqrt{m}}\right]\beta \tag{5.25}$$

For positive energy, this is exactly the kinetic operator found in [16]. The last term in Eq. (5.22) is a new result. The physics behind this term is not yet clear. However, the form of this operator resemble that of the spin-orbit interaction Hamiltonian (see Eq. (5.17)), that is

$$H_{s-o} = \frac{\lambda^4}{8m^2}\vec{\Sigma}\cdot\vec{p}\times\vec{E} - \frac{\lambda^4}{4m^2}\vec{\Sigma}\cdot\vec{E}\times\vec{p} \tag{5.26}$$

Notice too that the spin-orbit Hamiltonian is of fourth order in λ whereas h is of second order. It is possible to write h as

$$h = \frac{\lambda^2}{8m^2}\vec{\Sigma}\cdot\vec{p}\times(-i\vec{p}m)\beta - \frac{\lambda^2}{4m^2}\vec{\Sigma}\cdot(-i\vec{p}m)\times\vec{p}\beta \tag{5.27}$$

The first term is actually zero (as it is a curl of a gradient) but is added to make the comparison more obvious. Moreover, in the spherically symmetric case, assume the following:

$$m(\vec{r}) = m(r),\quad V(\vec{r}) = V(r),\quad \vec{A} = 0 \tag{5.28}$$

Then the operators in Eqs. (5.26) and (5.27) have the following almost similar forms:

$$h = \frac{\lambda^2}{4m^2}\frac{1}{r}\frac{dm}{dr}\vec{\Sigma}\cdot\vec{L}\beta \tag{5.29}$$

$$H_{s-o} = \frac{\lambda^4}{4m^2}\frac{1}{r}\frac{dV}{dr}\vec{\Sigma}\cdot\vec{L} \tag{5.30}$$

Finally, let me conclude this part by writing the Dirac equation up to order λ^2 (see Eq. (5.18)):

$$\frac{\lambda^2}{4}\left[\frac{1}{\sqrt{m}}\vec{p}\cdot\frac{1}{\sqrt{m}}\vec{p}+\vec{p}\cdot\frac{1}{\sqrt{m}}\vec{p}\frac{1}{\sqrt{m}}+\frac{i}{m^2}\vec{\sigma}\cdot(\vec{p}m)\times\vec{p}\right]\psi_+ = (\varepsilon - m)\psi_+ \tag{5.31}$$

$$-\frac{\lambda^2}{4}\left[\frac{1}{\sqrt{m}}\vec{p}\cdot\frac{1}{\sqrt{m}}\vec{p}+\vec{p}\cdot\frac{1}{\sqrt{m}}\vec{p}\frac{1}{\sqrt{m}}+\frac{i}{m^2}\vec{\sigma}\cdot(\vec{p}m)\times\vec{p}\right]\psi_- = (\varepsilon + m)\psi_- \tag{5.32}$$

Equation (5.31) implies the approximation statement that $\varepsilon \approx m + \lambda^2\tilde{E}$, where $\tilde{E}$ is the equivalent non-relativistic energy for the position-dependent mass system. The first of these two equations is to be compared with the Pauli equation without an interaction, which for the electron reads:

$$\frac{\lambda^2}{2m}\vec{p}^{\,2}\psi_+ = E\psi_+ \tag{5.33}$$

CHAPTER 6

CONCLUSION

In my thesis work, I studied four problems related to the Dirac equation. The first was an exact solution of the Dirac and Klein-Gordon equations coupled to scalar and vector potentials of equal magnitudes. The aim was to find the exact energy spectra and wave functions for three non-central potentials that include as limiting cases the following three known potentials: Coulomb, Oscillator and Hartmann. The Coulomb and Oscillator potentials were solved a long time ago by other means. I compared the energy spectra that I found for both potentials with those found previously by other well-established methods. It was found that both spectra did not agree with each other. However, when taking the non-relativistic limits both solutions agree. This is in accordance with the view that even though that the non-relativistic limit is unique, the relativistic results are not. These findings made it clear that exact solutions of the Dirac equation by the equal scalar-vector method must not be misinterpreted as relativistic generalizations of the corresponding non-relativistic problems.

In the second problem of this work, I studied the Klein-Gordon equation with unequal scalar and vector potentials. I took the s-wave Klein-Gordon-Morse problem. In this case I showed that by comparing the solution of this problem with the solution of the Dirac

equation for this potential, found in the recent literature, both solutions agree under certain physical constraints.

In the third problem, I returned to the Dirac equation with scalar and vector potentials. However, in this case I tackled what is called spin and pseudo spin symmetry problems. In these cases, the sum or difference between the scalar and the vector potentials was taken to be constant. These studies investigate exact solutions of the Dirac equation not as generalizations of non-relativistic potentials, but in studies related to nuclear structure and symmetry-breaking in nuclei. I showed that the solutions found in the first problem cited above give solutions for the second after shifting the mass by a constant.

In the last problem, I tackled the subject of the non-relativistic limit of the Dirac equation for a particle having position dependent mass and interacting with an electromagnetic field. I used two consecutive Fouldy-Wouthuysen transformations to cancel the odd operators in the Dirac equation to fourth power in the Compton wavelength (1/c). At the end, I wrote an expression for the kinetic operator. This operator is unique and can be used as the kinetic term in the Schrödinger equation. I also obtained a new term that was not mentioned previously in the literature. The physics of that term is not clear yet. However, I showed very clearly the similarity between this new term and the Hamiltonian for the spin-orbit interaction.

Many new issues and problems are still open in the realm of the Dirac equation. For example, exact solutions for the Dirac equation with position dependent mass are scarce in the literature. These are of course more profound than the approximate theory I

presented in this work. Another issue is how to use the different techniques, used in the solution of non-relativistic problems, in the domain of the Dirac equation. Two such examples are the relativistic extension of the method of complex scaling and the relativistic J-matrix method in scattering calculations. These are some problems that are under investigation.

APPENDIX

SPECIAL FUNCTIONS

This appendix contains a collection of properties of special functions of theoretical physics that are used frequently in this thesis. Moreover, it may also be of use in other works. General references for this appendix are to be found in [45].

1. The Gamma $(\Gamma(x))$ **and Beta Functions** $(B(x, y))$

$$\text{i) } \Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt \quad \text{Re}(x) > 0 ; \; B(x, y) = \int_0^1 t^{x-1} (1-t)^{y-1} dt \quad \text{Re}(x) > 0, \text{Re}(y) > 0 \tag{A.1}$$

$$\text{ii) } \Gamma(x+1) = x\Gamma(x) ; \;\; \Gamma(1) = 1 ; \;\; \Gamma(1/2) = \sqrt{\pi} ; \;\; \Gamma(n+1) = n! ; \;\; n = \text{non - negative integer} \tag{A.2}$$

$$\text{iii) } B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \tag{A.3}$$

$$\text{iv) } \Gamma(m) = \infty \text{ if } m = 0,-1,-2,... \tag{A.4}$$

2. Legendre Polynomials $P_n(x)$

$$\text{i) } P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n = \sum_{k=0}^{[n/2]} \frac{(-1)^k (2n-2k)!}{2^k k!(n-k)!(n-2k)!} x^{n-2k} \;\; , \; x \in [-1, 1] , \; n = 0,1,2,... \tag{A.5}$$

$$\text{ii) } \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n \;\; , \; |t| < 1 \tag{A.6}$$

$$\text{iii) } (1-x^2) P_n(x)'' - 2x P_n(x)' + n(n+1) P_n(x) = 0 \tag{A.7}$$

$$\text{iv) } P_{2n}(0) = (-1)^n \frac{(2n)!}{2^{2n} (n!)^2} ; \; P_{2n+1}(0) = 0 ; \; P_n(\pm 1) = (\pm 1)^n \tag{A.8}$$

v) $P_n(x) = \frac{1}{\pi}\int_0^{\pi}\left[x+\sqrt{x^2-1}\cos\varphi\right]^n d\varphi$ (A.9)

vi) $xP_n(x) = \frac{n+1}{2n+1}P_{n+1}(x) + \frac{n}{2n+1}P_{n-1}(x)$ (A.10)

vii) $(x^2-1)P_n(x)' = nxP_n(x) - nP_{n-1}(x)$ (A.11)

viii) $\int_{-1}^{+1} P_n(x)P_m(x)dx = \frac{2}{2n+1}\delta_{nm}$ (A.12)

3. Associated Legendre Functions $P_n^m(x)$

i) $P_n^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x)$, $x\in[-1,1]$ (A.13)

ii) $(1-x^2)P_n^m(x)'' - 2xP_n^m(x)' + \left\{n(n+1) - \frac{m^2}{1-x^2}\right\}P_n^m(x) = 0$ (A.14)

iii) $P_n^{m+1}(x) - \frac{2mx}{\sqrt{1-x^2}}P_n^m(x) + \{n(n+1)-m(m-1)\}P_n^{m-1}(x) = 0$ (A.15)

iv) $(2n+1)xP_n^m(x) = (n+m)P_{n-1}^m(x) + (n-m+1)P_{n+1}^m(x)$ (A.16)

v) $Y_l^{(m)}(\theta,\varphi) = (-1)^m\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P_l^{|m|}(\cos\theta)e^{im\varphi}$ (Spherical Harmonics) (A.17)

vi) $\int_{-1}^{+1} P_n^m(x)P_{n'}^m(x)dx = \frac{2(n+m)!}{(2n+1)(n-m)!}\delta_{nn'}$ (A.18)

4. Hermite Polynomials $H_n(x)$

i) $H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2} = \sum_{k=0}^{[n/2]}\frac{(-1)^k n!}{k!(n-2k)!}(2x)^{n-2k}$, $x\in(-\infty,\infty)$, $n = 0,1,2,...$ (A19)

ii) $e^{2xt-t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^2$ (A.20)

iii) $H_n(x)'' - 2xH_n(x)' + 2nH(x) = 0$ (A.21)

iv) $H_{2n}(0) = (-1)^n \frac{(2n)!}{n!}$; $H_{2n+1}(0) = 0$ (A.22)

v) $H_n(x) = \frac{2^n (-i)^n e^{x^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-t^2+2itx} t^n dt$ (A.23)

vi) $H_n(x)' = 2nH_{n-1}(x) \quad (n \geq 1)$, $H_0(x)' = 0$ (A.24)

vii) $xH_n(x) = \frac{1}{2} H_{n+1}(x) + nH_{n-1}(x) \quad (n \geq 1)$, $H_1(x) = 2xH_0(x)$ (A.25)

viii) $\int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi} \delta_{nm}$ (A.26)

6. Laguerre Polynomials $L_n(x)$

i) $L_n(x) = \frac{1}{n!} e^x \frac{d^n}{dx^n} \left(e^{-x} x^n \right) = \sum_{k=0}^{n} \frac{(-1)^k n!}{(k!)^2 (n-k)!} x^k$, $x \in [0, \infty)$, $n = 0,1,2,...$ (A.27)

ii) $(1-t)^{-1} e^{-xt/(1-t)} = \sum_{n=0}^{\infty} L_n(x) t^n$, $|t| < 1$ (A.28)

iii) $xL_n(x)'' + (1-x)L_n(x)' + nL_n(x) = 0$ (A.29)

iv) $L_n(0) = 1$, $L_n(0)' = -n$ (A.30)

v) $xL_n(x)' = nL_n(x) - nL_{n-1}(x) \quad (n \geq 1)$, $L_0(x)' = 0$ (A.31)

vi) $xL_n(x) = (2n+1)L_n(x) - nL_{n-1}(x) - (n+1)L_{n+1}(x) \quad (n \geq 1)$, $L_1(x) = (1-x)L_0(x)$ (A.32)

viii) $\int_0^\infty e^{-x} L_n(x) L_m(x) dx = \delta_{nm}$ (A.33)

6. Associated Laguerre Polynomials $L_n^\alpha(x)$

i) $L_n^\alpha(x) = \frac{x^{-\alpha}}{n!} e^x \frac{d^n}{dx^n}\left(e^{-x} x^{n+\alpha}\right) = \sum_{k=0}^{n} \frac{(-1)^k \Gamma(n+\alpha+1)}{k!(n-k)!\Gamma(k+\alpha+1)} x^k$, $x \in [0,\infty)$, $\alpha > -1$,

$n = 0, 1, 2, ...$

(A.34)

ii) $(1-t)^{-\alpha-1} e^{-xt/(1-t)} = \sum_{n=0}^{\infty} L_n^\alpha(x) t^n$, $|t| < 1$ (A.35)

iii) $x L_n^\alpha(x)'' + (\alpha+1-x) L_n^\alpha(x)' + n L_n^\alpha(x) = 0$ (A.36)

iv) $L_n^\alpha(0) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1}$ (A.37)

v) $x L_n^\alpha(x)' = -x L_{n-1}^{\alpha+1}(x) = n L_n^\alpha(x) - (n+\alpha) L_{n-1}^\alpha(x)$ $(n \geq 1)$, $L_0^\alpha(x)' = 0$ (A.38)

vi) $x L_n^\alpha(x) = (2n+\alpha+1) L_n^\alpha(x) - (n+\alpha) L_{n-1}^\alpha(x) - (n+1) L_{n+1}^\alpha(x)$ $(n \geq 1)$,

$L_1^\alpha(x) = (1+\alpha-x) L_0^\alpha(x)$; $L_n^{\alpha+1}(x) - L_{n-1}^{\alpha-1}(x) = L_n^\alpha(x)$ (A.39)

viii) $\int_0^\infty e^{-x} x^\alpha L_n^\alpha(x) L_m^\alpha(x) dx = \frac{\Gamma(n+\alpha+1)}{n!} \delta_{nm}$ (A.40)

7. Chebyshev Polynomials $T_n(x)$ **and** $U_n(x)$

i) $T_n(x) = \cos\left(n \cos^{-1} x\right)$ (Chebyshev Polynomials of first kind)

$U_n(x) = \sin\left(n \cos^{-1} x\right)$ (Chebyshev Polynomials of second kind), $x \in [-1, 1]$,

$n = 0,1,2,...$ (A.41)

ii) $T_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!}{(2k)!(n-2k)!} (1-x^2)^k x^{n-2k}$

$$U_n(x) = \sum_{k=0}^{[(n-1)/2]} \frac{(-1)^k n!}{(2k+1)!(n-2k-1)!} (1-x^2)^{k+1/2} x^{n-2k-1} \quad \text{(A.42)}$$

iii) $(1-x^2)T_n(x)'' - xT_n(x)' + n^2 T_n(x) = 0$

$$(1-x^2)U_n(x)'' - xU_n(x)' + n^2 U_n(x) = 0 \quad \text{(A.43)}$$

iv) $\frac{1-t^2}{1-2tx+t^2} = T_0(x) + 2\sum_{n=1}^{\infty} T_n(x) t^n$

$$\frac{\sqrt{1-x^2}}{1-2tx+t^2} = \sum_{n=1}^{\infty} U_{n+1}(x) t^n \ , \ U_0(x) = 0 \quad \text{(A.44)}$$

v) $T_n(\pm 1) = (\pm 1)^n$, $T_{2n}(0) = (-1)^n$, $T_{2n+1}(0) = 0$

$$U_n(\pm 1) = 0 \, , \quad T_{2n}(0) = 0 \, , \quad T_{2n+1}(0) = (-1)^n \quad \text{(A.45)}$$

vi) $xT_n(x) = \frac{1}{2} T_{n+1}(x) + \frac{1}{2} T_{n-1}(x)$ $(n \geq 1)$, $T_1(x) = xT_0(x)$

$$xU_n(x) = \frac{1}{2} U_{n+1}(x) + \frac{1}{2} U_{n-1}(x) \ (n \geq 1) \, , \ U_1(x) = \sqrt{1-x^2} \ , \ T_0(x) = 0 \quad \text{(A.46)}$$

vii) $(1-x^2)T_n(x)' = -nxT_n(x) + nT_{n-1}(x)$ $(n \geq 1)$

$$(1-x^2)U_n(x)' = -nxU_n(x) + nU_{n-1}(x) \ (n \geq 1) \quad \text{(A.47)}$$

viii) $$\int_{-1}^{+1} \frac{T_n(x) T_m(x)}{\sqrt{1-x^2}} dx = \begin{cases} 0 & n \neq m \\ \pi/2 & n = m \neq 0 \\ \pi & n = m = 0 \end{cases}$$

$$\int_{-1}^{+1}\frac{U_n(x)U_m(x)}{\sqrt{1-x^2}}dx=\begin{cases}0 & n\neq m\\ \pi/2 & n=m\neq 0\\ 0 & n=m=0\end{cases} \tag{A.48}$$

8. Gegenbauer Polynomials $C_n^{\lambda}(x)$

i) $C_n^{\lambda}(x)=\sum_{k=0}^{[n/2]}\frac{(-1)^k\Gamma(n-k+\lambda)}{k!(n-2k)!\Gamma(\lambda)}(2x)^{n-2k}$, $x\in[-1,1]$, $\lambda>-1/2$, $n=0,1,2,...$ (A.49)

ii) $\frac{1}{\left(1-2xt+t^2\right)^{\lambda}}=\sum_{n=0}^{\infty}C_n^{\lambda}(x)t^2$, $|t|<1$ (A.50)

iii) $(1-x^2)C_n^{\lambda}(x)''-(2\lambda+1)xC_n^{\lambda}(x)'+n(n+2\lambda)C_n^{\lambda}(x)=0$ (A.51)

iv) $C_n^{\lambda}(x)'=2\lambda C_{n+1}^{\lambda+1}(x)$ (A.52)

v) $xC_n^{\lambda}(x)=\frac{2\lambda+n-1}{2(\lambda+n)}C_{n-1}^{\lambda}(x)+\frac{n+1}{2(\lambda+n)}C_{n+1}^{\lambda}(x)$ $(n\geq 1)$

$nC_n^{\lambda}(x)=2\lambda xC_{n-1}^{\lambda+1}(x)-2\lambda C_{n-2}^{\lambda+1}(x)$ $(n\geq 2)$

$(n+2\lambda)C_n^{\lambda}(x)=2\lambda xC_n^{\lambda+1}(x)-2\lambda xC_{n-1}^{\lambda+1}(x)$ $(n\geq 1)$

$nC_n^{\lambda}(x)=(n-1+2\lambda)xC_{n-1}^{\lambda}(x)-2\lambda(1-x^2)C_{n-2}^{\lambda-1}(x)$ $(n\geq 2)$ (A53)

viii) $\int_0^{\infty}(1-x^2)^{\lambda-1/2}C_n^{\lambda}(x)C_m^{\lambda}(x)dx=2^{1-2\lambda}\pi\frac{\Gamma(n+2\lambda)}{(n+\lambda)[\Gamma(\lambda)]^2 n!}\delta_{nm}$ (A.54)

9. Jacobi Polynomials $P_n^{(\alpha,\beta)}(x)$

i) $P_n^{(\alpha,\beta)}(x)=\sum_{k=0}^{n}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(k+\alpha+1)\Gamma(n+\beta-k+1)(n-k)!k!}\left(\frac{x-1}{2}\right)^k\left(\frac{x+1}{2}\right)^{n-k}$

$$= \sum_{k=0}^{n} \frac{\Gamma(n+\alpha+1)\Gamma(n+k+\alpha+\beta+1)}{\Gamma(k+\alpha+1)\Gamma(n+\alpha+\beta+1)(n-k)!k!}\left(\frac{x-1}{2}\right)^k$$

$$= \sum_{k=0}^{n} \frac{(-1)^{n-k}\Gamma(n+k+\alpha+\beta+1)\Gamma(n+\beta+1)}{\Gamma(k+\beta+1)\Gamma(n+\alpha+\beta+1)(n-k)!k!}\left(\frac{x+1}{2}\right)^k , \ x \in [-1,1] \qquad \text{(A.55)}$$

ii)

$$\frac{2^{\alpha+\beta}}{(1-2xt+t^2)^{1/2}\{1-t+(1-2xt+t^2)^{1/2}\}^{\alpha}\{1+t+(1-2xt+t^2)^{1/2}\}^{\beta}} = \sum_{n=0}^{\infty} P_n^{(\alpha,\beta)}(x)t^n \quad \text{(A.56)}$$

iii) $(1-x^2)P_n^{(\alpha,\beta)}(x)'' + \{\beta-\alpha-(\alpha+\beta+2)x\}P_n^{(\alpha,\beta)}(x)' + n(n+\alpha+\beta+1)P_n^{(\alpha,\beta)}(x) = 0$ (A57)

iv)

$$2n(\alpha+\beta+n)(\alpha+\beta+2n-2)P_n^{(\alpha,\beta)}(x) = (\alpha+\beta+2n-1)\cdot$$
$$\{\alpha^2-\beta^2+(\alpha+\beta+2n)(\alpha+\beta+2n-2)x\}P_{n-1}^{(\alpha,\beta)}(x) - 2(\alpha+n-1)(\beta+n-1)(\alpha+\beta+2n)P_{n-2}^{(\alpha,\beta)}(x)$$

$$(\alpha+\beta+2n)P_n^{(\alpha,\beta-1)}(x) = (\alpha+\beta+n)P_n^{(\alpha,\beta)}(x) + (\alpha+n)P_{n-1}^{(\alpha,\beta)}(x)$$

$$(\alpha+\beta+2n)P_n^{(\alpha-1,\beta)}(x) = (\alpha+\beta+n)P_n^{(\alpha,\beta)}(x) - (\beta+n)P_{n-1}^{(\alpha,\beta)}(x) \qquad \text{(A.58)}$$

v) $P_n^{(\alpha,\beta)}(x)' = \frac{1}{2}(1+\alpha+\beta+n)P_{n-1}^{(\alpha+1,\beta+1)}(x)$

$$(x+1)P_n^{(\alpha,\beta)}(x)' = nP_n^{(\alpha,\beta)}(x) + (\beta+n)P_{n-1}^{(\alpha+1,\beta)}(x)$$

$$(x-1)P_n^{(\alpha,\beta)}(x)' = nP_n^{(\alpha,\beta)}(x) - (\alpha+n)P_{n-1}^{(\alpha,\beta+1)}(x)$$

$$P_n^{(\alpha,\beta)}(x)' = \frac{1}{2}(n+\beta)P_{n-1}^{(\alpha+1,\beta)}(x) + \frac{1}{2}(n+\alpha)P_{n-1}^{(\alpha+1,\beta+1)}(x) \qquad \text{(A.59)}$$

vi) $\int_{-1}^{+1}(1-x)^{\alpha}(1+x)^{\beta}P_n^{(\alpha,\beta)}(x)P_m^{(\alpha,\beta)}(x)=\frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)n!\Gamma(n+\alpha+\beta+1)}\delta_{nm}$ (A60)

10. Bessel Functions $J_q(x)$, $Y_q(x)$

i) $J_q(x)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(n+k+1)!}\left(\frac{x}{2}\right)^k$, $Y_q(x)=\frac{\cos q\pi J_q(x)-J_{-q}(x)}{\sin q\pi}$ $x\in(-\infty,\infty)$ (A.61)

ii) $\exp\left\{\frac{1}{2}x\left(t-\frac{1}{t}\right)\right\}=\sum_{n=0}^{\infty}J_n(x)t^n$ (A.62)

iii) $J_n(x)=\frac{1}{\pi}\int_0^{\pi}\cos(n\varphi-x\sin\varphi)d\varphi$ (A.63)

iv) $x^2J_q(x)''+xJ_q(x)'+(x^2-q^2)J_q(x)=0$

$x^2Y_q(x)''+xY_q(x)'+(x^2-q^2)Y_q(x)=0$ (A.64)

v) $\frac{d}{dx}\{x^nJ_n(x)\}=x^nJ_{n-1}(x)$, $\frac{d}{dx}\{x^{-n}J_n(x)\}=-x^{-n}J_{n+1}(x)$ (A.65)

vi) $\frac{2n}{x}J_n(x)=J_{n-1}(x)+L_{n+1}(x)$ (A.66)

vii) $j_l(x)=\sqrt{\frac{\pi}{2x}}J_{l+1/2}(x)$, $y_l(x)=\sqrt{\frac{\pi}{2x}}Y_{l+1/2}(x)$ (A.67)

viii) $\int_0^a xJ_n(\xi_i x)J_n(\xi_j x)dx=\frac{a^2}{2}\{J_{n+1}(\xi_i a)\}^2\delta_{ij}$, $J_n(\xi a)=0$

$\int_{-\infty}^{\infty}j_n(x)j_m(x)dx=\frac{\pi}{2n+1}\delta_{nm}$ (A.68)

11. Generalized Hypergeometric Functions ${}_mF_n(\alpha_1,\alpha_2,....\alpha_m;\beta_1,\beta_2,....\beta_n;x)$

$${}_mF_n(\alpha_1,\alpha_2,....\alpha_m;\beta_1,\beta_2,....\beta_n;x)=\sum_{k=0}^{\infty}\frac{(\alpha_1)_k(\alpha_2)_k...(\alpha_m)_k}{(\beta_1)_k(\beta_2)_k...(\beta_n)_k}\frac{x^k}{k!},\ x\in(-\infty,\infty) \tag{A.69}$$

$$(\alpha)_k=\frac{\Gamma(\alpha+k)}{\Gamma(\alpha)},\quad (\alpha)_0=1 \tag{A.70}$$

12. The Hypergeometric Function ${}_2F_1(a,b;c;x)$

i) $${}_2F_1(a,b;c;x)=\sum_{k=0}^{\infty}\frac{(a)_k(b)_k}{(c)_k}\frac{x^k}{k!},\ x\in(-\infty,\infty) \tag{A.71}$$

ii) $${}_2F_1(a,b;c;x)=\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-xt)^{-a}\,dt \tag{A.72}$$

iii) $$x(1-x)\,{}_2F_1(a,b;c;x)''+[c-(a+b+1)x]\,{}_2F_1(a,b;c;x)'-ab\,{}_2F_1(a,b;c;x)=0 \tag{A.73}$$

iv) $$(c-a-b)\,{}_2F_1(a,b;c;x)+a(1-x)\,{}_2F_1(a+1,b;c;x)-(c-b)\,{}_2F_1(a,b-1;c;x)=0$$

$$(c-a-1)\,{}_2F_1(a,b;c;x)+a\,{}_2F_1(a+1,b;c;x)-(c-1)\,{}_2F_1(a,b;c-1;x)=0$$

$$c(1-x)\,{}_2F_1(a,b;c;x)-c\,{}_2F_1(a-1,b;c;x)+(c-b)x\,{}_2F_1(a,b;c+1;x)=0 \tag{A.74}$$

v) $$\frac{d^m}{dx^m}\,{}_2F_1(a,b;c;x)=\frac{(a)_m(b)_m}{(c)_m}\,{}_2F_1(a+m,b+m;c+m;x) \tag{A.75}$$

13. The Confluent Hypergeometric Function ${}_1F_1(a;b;x)$

i) $${}_1F_1(a;b;x)=\sum_{k=0}^{\infty}\frac{(a)_k}{(b)_k}\frac{x^k}{k!},\ x\in(-\infty,\infty) \tag{A.76}$$

ii) $${}_1F_1(a;b;x)=\frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)}\int_0^1 t^{a-1}(1-t)^{b-a-1}e^{xt}\,dt,\quad a>0,\ b>0 \tag{A.77}$$

iii) $x\,{}_1F_1(a;b;x)'' + (b-x)\,{}_1F_1(a;b;x)' - a\,{}_1F_1(a;b;x) = 0$ (A.78)

iv) $(b-a-1)\,{}_1F_1(a;b;x) + a\,{}_1F_1(a+1;b;x) - (b-1)\,{}_1F_1(a;b-1;x) = 0$

$b\,{}_1F_1(a;b;x) - b\,{}_1F_1(a-1;b;x) - x\,{}_1F_1(a;b+1;x) = 0$

$(a-1+x)\,{}_1F_1(a;b;x) + (b-a)\,{}_1F_1(a-1;b;x) - (b-1)x\,{}_1F_1(a;b-1;x) = 0$

$b(a+x)\,{}_1F_1(a;b;x) - ab\,{}_1F_1(a+1;b;x) - (b-a)\,{}_1F_1(a;b+1;x) = 0$

$(b-a)\,{}_1F_1(a-1;b;x) + (2a-b+x)\,{}_1F_1(a;b;x) - a\,{}_1F_1(a+1;b;x) = 0$

$b(b-1)\,{}_1F_1(a;b-1;x) - b(b-1+x)\,{}_1F_1(a;b;x) + (b-a)x\,{}_1F_1(a;b+1;x) = 0$ (A.79)

v) $\dfrac{d^m}{dx^m}\,{}_1F_1(a;b;x) = \dfrac{(a)_m}{(b)_m}\,{}_1F_1(a+m;b+m;x)$ (A.80)

14. Relationships between Different Functions and the Hypergeometric ones

i) $P_n(x) = {}_2F_1\left(-n, n+1; 1; \dfrac{1-x}{2}\right)$ (A.81)

ii) $P_n^m(x) = \dfrac{(n+m)!}{(n-m)!}\dfrac{(1-x^2)^{m/2}}{2^m m!}\,{}_2F_1\left(m-n, m+n+1; m+1; \dfrac{1-x}{2}\right)$ (A.82)

iii) $J_n(x) = \dfrac{e^{-ix}}{n!}\left(\dfrac{x}{2}\right)^n\,{}_1F_1(n+1/2; 2n+1; x)$ (A.83)

iv) $H_{2n}(x) = (-1)^n\dfrac{(2n)!}{n!}\,{}_1F_1(-n; 1/2; x^2)$ (A.84)

v) $H_{2n+1}(x) = (-1)^n\dfrac{2(2n+1)!}{n!}x\,{}_1F_1(-n; 3/2; x^2)$ (A.85)

vi) $L_n(x) = {}_1F_1(-n; 1; x)$ (A.86)

vii) $L_n^k(x) = \frac{\Gamma(n+k+1)}{n!\Gamma(k+1)} {}_1F_1(-n; k+1; x)$ (A.87)

viii) $T_n(x) = {}_2F_1(-n; n; 1/2; \frac{1-x}{2})$ (A.88)

ix) $U_n(x) = \sqrt{1-x^2}\, n\, {}_2F_1(-n+1; n+1; 3/2; \frac{1-x}{2})$ (A.89)

x) $C_n^{\lambda}(x) = \frac{\Gamma(n+2\lambda)}{n!\Gamma(2\lambda)} {}_2F_1(-n; n+2\lambda; \lambda+1/2; \frac{1-x}{2})$ (A.90)

xi) $P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)} {}_2F_1(-n; n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2})$ (A.91)

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